iGeoT v1.0:
Automatic Parameter Estimation for Multicomponent Geothermometry

User's Guide

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1. INTRODUCTION

GeoT [*Spycher et al*., 2016a; http://eesa.lbl.gov/technology/geot/] implements the multicomponent geothermometry method developed by *Reed and Spycher* [1984] into a stand-alone computer program to ease the application of this method and to improve the prediction of geothermal reservoir temperatures using full and integrated chemical analyses of geothermal fluids. Reservoir temperatures are estimated from statistical analyses of mineral saturation indices computed as a function of temperature. The reconstruction of the deep geothermal fluid compositions, and geothermometry computations, are all implemented into the same computer program, allowing unknown or poorly constrained input parameters to be estimated by numerical optimization. This integrated geothermometry approach presents advantages over classical geothermometers for fluids that have not fully equilibrated with reservoir minerals and/or that have been subject to processes such as dilution and gas loss. Integrated multicomponent solute geothermometry is described in *Spycher et al.* [2014, 2016a and 2016b].

Figure 1 shows the structure of GeoT and an example computation, illustrating the clustering of mineral saturation lines at the equilibrium point log(Q/K)=0, where statistical measures attain their minimum, indicating the inferred reservoir temperature.
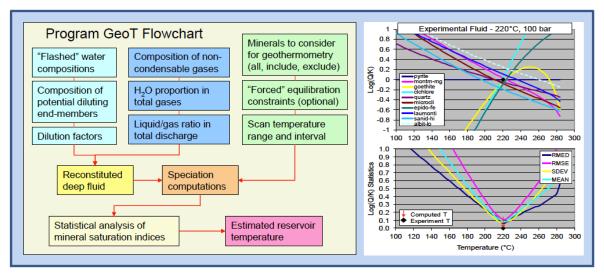
Figure 1. Structure of the geothermometry program GeoT and example computations.

GeoT's multicomponent geothermometry has been integrated into the iTOUGH2 simulation-optimization framework to automatically estimate some of GeoT's input parameters (e.g., steam weight fractions, concentration/dilution factors, input concentrations of aqueous and gas species) by minimizing the statistical measures that describe the clustering of mineral saturation indices near zero. iTOUGH2 (http://esd.lbl.gov/iTOUGH2) is a computer program for parameter estimation, sensitivity analysis, and uncertainty propagation analysis [*Finsterle*, 2007a, b, c]. It contains a number of local and global minimization algorithms for automatic calibration of a model against measured data, or for the solution of other optimization problems (such as the minimization of clustering measures of saturation indices around zero).

The combination of iTOUGH2 and GeoT is referred to as iGeoT. This stand-alone iGeoT program can be run in three modes:

- *Forward Mode* (no parameter estimation) – In this case iGeoT runs just like GeoT, providing reservoir temperature estimations from known (or independently estimated) input values of solute concentrations, steam fraction, gas concentrations, and dilution factor.

- *Automatic Mode* – With this option, unknown or poorly constrained parameters such the concentrations of specific solutes (e.g., Al, Mg) or gases, steam fraction, and dilution factor are estimated by numerical optimization. The user flags in the standard GeoT input file (using the special character @, Section 4.5) which of its input parameters shall be considered uncertain and thus estimated by numerical optimization. In *Automatic Mode*, iGeoT automatically sets up a suitable iTOUGH2 command file with instructions for the optimization. In this mode, the user has access to iTOUGH2 optimization without the need to be proficient in the use of iTOUGH2. Moreover, the iTOUGH2 command file automatically generated by iGeoT can be used as a template for further analyses to be conducted in *Expert Mode*.

- *Expert Mode* – This option is similar to the *Automatic Mode*, except that the user controls the optimization by supplying a command file containing standard iTOUGH2 instructions. In this mode, the user has access to all options for specifying inputs, selecting algorithms, and performing additional analyses (e.g., sensitivity and uncertainty quantification analyses).

This manual contains installation instructions for iGeoT, and briefly describes the input formats needed to run iGeoT in Automatic or Expert Mode. An example is also provided to demonstrate the use of iGeoT. For details about the theory and usage of GeoT and iTOUGH2, the reader is referred to *Spycher et al.* [2016a,b] and *Finsterle* [2007a,b,c], respectively.

2. INSTALLATION AND EXECUTION

3.1 Distribution Licenses

iGeoT is currently distributed as end-use, executable binary files suitable for either Windows, Mac, or Unix/Linux platforms. Section 3.2 provides instructions on how to install and run this software.

3.2 Installing and Running iGeoT

This program is command-driven and therefore must be run from a command window. To install the program, simply unzip the provided compressed file into a folder of your choice. Prior to running iGeoT, make sure to read any *readme* files associated with the distribution subfolders, as well as the GeoT v2.1 User's Guide [*Spycher et al.*, 2016a] provided in the *Documentation* subfolder. You can then proceed to run the examples discussed in Section 5.

To run iGeoT, copy into a folder of your choice (e.g., *run_folder*): 1) the GeoT input files as described below, 2) the thermodynamic database file (e.g., *tk-slt.h06_jun16.dat*) and 3) the executable file suitable for your platform (which can be found in the *Executable* subfolder). Alternatively, copy the executable and/or related script/batch files into a separate folder (e.g., *bin*) and add the name of this directory to the command search path for your platform (e.g., environment variable PATH in Windows). Then change directory to the run folder, and follow the instructions given below.

Running iGeoT under Unix, Linux, and MacOS

(1) To run iGeoT in forward mode, i.e., without parameter estimation, type the name of the executable file at the command prompt. You will be prompted for the GeoT input file name (by default *geot.inp*) then for the name of a file with inputs related to parameter estimation (by default *igeot.inp*). In this case (forward mode), *igeot.inp* is an empty dummy file.

(2) To run iGeoT with parameter estimation in Automatic Mode, at the command prompt type the name of the executable file as described above for (1), but provide a parameter estimation input file (by default *igeot.inp*) with keyword AUTOMATIC on the first line of the file and indicate the parameters to be estimated in the GeoT input file by flagging them with the special character '@', as described in Section 4.5.

(3) To run iGeoT with parameter estimation in Expert Mode, follow the same steps as in (1), but provide optimization instructions in the parameter input file (by default *igeot.inp*).

Alternatively, the program can be run by using Unix shell script file *geot* (for forward runs) or *igeot* (for inverse runs in Automatic and Expert model). Both Unix shell script files can be found in distribution subfolder *Scripts*. The names of input files are provided on the command line, for example:

```
geot geot.inp
igeot igeot.inp geot.inp
```

<u>Running under Windows</u>

(1) To run GeoT in forward mode, i.e., without parameter estimation, type the name of the executable file at the command prompt. You will be prompted for the GeoT input file name (by default *geot.inp*) then for the name of a file with inputs related to parameter estimation (by default *igeot.inp*), which in this case must be present in the current folder but can be empty (dummy file).

Note, double-clicking on the executable file will also run the program. However, using the command line is recommended, because potential error messages printed to screen will not be visible when double-clicking the executable.

(2) To run iGeoT with parameter estimation in Automatic Mode, type the name of the executable file as described above for (1), but provide a parameter estimation input file (by default *igeot.inp*) with keyword AUTOMATIC on the first line and indicate the parameters to be estimated in the GeoT input file by flagging them with the special character '@', as described in Section 4.5.

(3) To run iGeoT with parameter estimation in Expert Mode, follow the same steps as in (1), but provide iGeoT optimization instructions in the parameter input file (by default *igeot.inp*)

(4) Alternatively, the program can be run by using batch file *geot.bat* (for forward runs) or *igeot.bat* (for inverse runs in Automatic and Expert model). Both batch files can be found in distribution subfolder *Scripts*. The names of input files are provided on the command line of a DOS command prompt window, for example:

```
geot geot.inp
igeot igeot.inp geot.inp
```

3. THE GEOT FORWARD OPERATOR

3.1 General Concept

iGeoT provides inverse modeling capabilities for GeoT to estimate input parameters other than temperature (e.g., steam fraction, dilution factor). In this context, GeoT is considered the forward operator. It is important to note that GeoT, by itself (i.e., without iGeoT) solves a minimization problem to estimate reservoir temperature. GeoT does this by evaluating mineral saturation indices, $\log(Q/K)$, over a user-specified temperature range at temperatures separated by a constant interval ΔT. For example, the saturation indices for a set of reservoir minerals are calculated every 1°C between 100°C and 300°C. At each evaluated temperature point, the clustering of saturation indices near zero (indicating equilibrium) is evaluated using several statistical measures. The point where the clustering measure is at its minimum is considered the likely reservoir temperature.

Prior to computing saturation indices, the composition of the deep fluid is reconstructed by applying corrections for any dilution and/or mixing effects and by numerically adding back (to the analyzed fluid composition) any gases that may have exsolved from the deep fluid on its way to the ground surface. However, the input parameters necessary to reconstruct the deep fluid composition may be uncertain or unknown. These parameters (in particular steam weight fractions, concentration/ dilution factors, and input concentrations) can be estimated by adjusting them to maximize the clustering of mineral saturation indices near zero. It is this latter inverse problem that is solved by iGeoT.

iGeoT V1.0 is based on GeoT V2.1, which in turn is an updated version of the first released GeoT V1.4 version. The following sections summarize upgrades made to GeoT since its initial release.

3.2 GeoT V2.1 implemented into iGeoT V1.0

GeoT V2.1 is fully documented in *Spycher et al*. [2016a]. The upgrades since the previously released version V1.5, summarized below, include addition of new capabilities, improvements in user features, and bug fixes; all upgrades are backwards compatible.

- *New Capability – Mineral/Gas Reaction*

    Minerals and/or gases can be equilibrated with the solution by reaction (i.e., not by just fixing the concentration of one aqueous species to yield equilibrium, but by fully reacting a gas/mineral assemblage to bring it at equilibrium with the solution, at each temperature step, thus with re-computation of the concentrations of all aqueous species involved in the reaction).

    This capability is enabled by entering a non-zero integer following the mineral name (on the same record) in the input file. GeoT will then proceed to compute speciation and mineral saturation indices, first without reaction, as with previous code versions, using constraints, if any, set using *icon* ≠ 1. These initial speciation computations are then repeated, this time with reaction of the flagged minerals, and at all temperatures. If any constraints (*icon* ≠ 1) are specified in the input file, these are used for the initial speciation

calculations, then removed for subsequent speciation/reaction calculations if the constraint conflicts with a reaction (e.g., charge balance on HCO3- cannot be specified while reacting calcite; or Al cannot be constrained with albite while reacting this mineral).

Gases can be reacted with the solution in the same manner, with or without reacting minerals. This capability is enabled by entering, following the gas concentration (same record), a non-blank value corresponding to the logarithm (base 10) of the desired gas fugacity. Doing so forces reaction at equilibrium with the specified gas(es) at their specified fugacities, at all temperature steps.

- *New Capability – Iterative Estimation of Steam Fraction*

This option is enabled by entering a value of 1 or greater for the steam fraction (*stwf*). The entered value must correspond to the solution sampling pressure in bar.

When this option is enabled, GeoT estimates the steam fraction (*stwf*) by assuming iso-enthalpic boiling, starting at the estimated reservoir temperature, using pure water properties. This is done iteratively, by first estimating a reservoir temperature for a case with gases added back into solution assuming 1% steam fraction. A new steam fraction is then computed for iso-enthalpic boiling from the estimated temperature at the saturation pressure of pure water, down to the input sampling pressure (using pure-water liquid and vapor enthalpy data). The solution composition is then corrected using the new calculated steam fraction, and the reservoir temperature is estimated again for this new solution composition; a new steam fraction is then estimated for the new estimated temperature, and so on. This iterative procedure proceeds as long as the clustering of mineral saturation indices near zero improves (computed as the spread in the equilibration temperatures of all minerals considered in the temperature estimation). A maximum of 10 iterations is allowed.

This option should be used only with fluids from wells or from boiling springs (near 100°C) for which the assumption of iso-enthalpic boiling can be presumed reasonable. If this is not the case, the steam fraction is preferably estimated using iGeoT.

- *Improvement – Inclusion of Gases*

Gases can be included in the simulations without necessarily specifying a gas composition. When gas names are not followed by a concentration, the gases are included in the computation (i.e., their fugacity/saturation indices are computed), but the gases are not added back to the solution composition (i.e., same effect as specifying *stwf*=0). The gas saturation pressure of the solution and the gas fugacity coefficients are also output after initialization.

- *Improvement – Final Speciation Calculation*

A new printout parameter is read (optionally) in the input file, *iprt_final*; it must be entered after *tincp*, on the same record. If a non-zero *iprt_final* value is entered, a "final" set of speciation/temperature calculations is run, this time using the (constant) water composition corresponding to the reconstructed total concentrations for all species computed at the estimated reservoir temperature. This option is useful when temperature estimations are run using constraints (e.g., fix Al with a silicate mineral) and/or reacting minerals at each

temperature step (thus with changing solution composition at each temperature step). In this case, computed saturation indices are zero at all temperatures for all reacting minerals and minerals used to constrain the concentration of some species. By re-running a "final" computation using the total concentrations computed at the estimated temperature, one can examine (and plot) the saturation indices for these minerals away from the estimated temperature, and get a "final" temperature estimation including these minerals. It should be noted that in most cases, this "final" temperature is the same as the previously estimated temperature. Results of this "final" run are output in separate files, named *geot-final.out* and *speciate-final.out*.

- *Improvements – Fixed activity at all temperatures*
  The pH or activity of any species can be fixed at all temperatures with a new ICON=7 option.

- *New input capabilities in V1.5 and above*

  - The format of the GeoT V2.1 input file is the same as that for GeoT V1.4 (thus fully backward compatible) except for addition of solution density (*soldens*) on the *water ID* record, and the option to add concentration units following the concentration values if these are not molal-based.

  - By default, all solute concentrations are assumed to be in moles, and the solvent (water) "concentration" is in kilograms.

  - The input moles of solute are internally divided by the input kilograms of water, with units of molality (moles/kg-water) then carried for the computations.

  - For total concentrations, the user has a choice of other input concentration units. This option is enabled by following the input concentrations by at least one blank, followed by one of the following strings (self explanatory, quotes are required where shown, case-insensitive):

    `'mg/L'`
    `'ug/L'`
    `'ppm'` (or `ppm`)
    `'ppb'` (or `ppb`)
    `'mmol/kg'`
    `'umol/kg'` (for micromolal)
    `'mmol/L'`
    `'umol/L'` (for micromolar)
    `'as'` (or `as`)

    After mass-based units, the string `"as"` followed by an element name (with or without quotes, case insensitive) can be entered to specify the name of the element for which the molecular weight will be used to convert concentrations to molal units. If not specified, the molecular weight of the input primary species (read in the thermodynamic database) will be used by default. For this option, hard-wired

(thermodynamic database independent) molecular weights are currently available for the following elements/compounds (use the exact same spelling, but case independent):

```
Si, SiO2, H4SiO4, C, CaCO3, CO3, CO2, HCO3, H2CO3, N, N2,
NH3, NH4, NO3, NO2, B, As, Sb, Mo, U, Ti, S, S2, HS, H2S,
Al, Fe
```

Figure 2 shows an example input record.

```
# ID tc keepic stwf cfact soldens pmix (1 to nmix)
Hveragerdi_W4 20.0 1 0.04 1.0 1.0
#name icon guess(molal) input(mol) constr. sat.
H+        3  1.00E-09    1.514E-09
H2O       1  1.00        1.00
Cl-       1  1.00E-07    109.5       ppm
SO4--     1  1.00E-07    43.7        'mg/l'
HCO3-     1  1.00E-07    74.20       ppm as CO2
HS-       1  1.00E-07    19200.      ppb as H2S
SiO2(aq)  1  1.00E-07    281000.     'ug/L' as SiO2
Al+++     1  1.00E-07    5.19        'umol/kg'
Ca++      1  1.00E-07    1.73        ppm
Mg++      1  1.00E-07    8.23E-08
Fe++      1  1.00E-07    1.43E-07
K+        1  1.00E-07    3.43E-04
Na+       1  1.00E-07    153300      'ug/l'
F-        1  1.00E-07    0.0959      'mmol/kg'
'*'
```

Figure 2. Example input record showing added flexibility in specifying solutes.

Other minor adjustments were made to iGeoT relative to older GeoT versions to improve its performance during an inversion. These include:

- The name of the GeoT input file can be arbitrary (i.e., it is not assumed to be *geot.inp*). The name of all GeoT output files (main output, speciation output, and run log files) have the chosen input file name followed by *.out*, *_spec.out*, and *_log.out*, respectively. If final speciation calculations are requested (*iprt_final* > 0), the suffixes *_final.out* and *_spec_final.out* are added to the file names.

- Screen prompts followed by keyboard input are disabled when running iGeoT under Unix/Linux/Mac, and screen output is redirected to a *.msg* file. It is recommended to include the string *BATCH* in the title record to suppress screen output.

- If *iprt_final* > 0, the clustering measures are evaluated based on the final speciation calculations (see Section 3.2).

- The temperature at which the saturation index crosses the zero line is calculated by linear interpolation between the two discrete temperature points (separated by *ΔT*) where the sign of $\log(Q/K)$ changes. Note that in GeoT versions prior to V2.1, the crossing temperature was given by the discrete value (with resolution *ΔT*) that represents the lower of the two temperatures between which the saturation index changes its sign. Since the temperature

spread *ΔT* (which is calculated based on the crossing temperature) is used as one of the clustering criteria, it is preferred to have a continuous (rather than discrete) value of the crossing temperature, so that derivative-based minimization algorithms can be employed for the inversion. Numerical tests indicate that linear interpolation provides an accurate estimate of the actual crossing temperature if *ΔT* is chosen reasonably small.

- Similarly, the temperatures at which the clustering measures (median, standard deviation, root mean square error, or average) reach their respective minima are calculated as continuous (rather than discrete) values by (a) fitting a parabola through the three discrete temperature points that encompass the minimum, and (b) determining the vertex of that fitted parabola.

- The output of the multicomponent geothermometer is restructured (see Figure 3), now showing the real-valued estimation temperatures for different criteria and associated clustering measures. A combined temperature estimate is also provided, which is the weighted average of the temperatures at the various cluster-measure minima; the weights are the inverses of the spread statistics (i.e., standard deviation of cross temperatures, median, RMSE, standard deviation, and average residuals at respective minima).

- Certain parameters can be labeled directly in the GeoT input file for automatic parameter estimation; see the discussion of iGeoT Automatic Mode in Section 4.5 below. The labeling is done by preceding or following (without spaces) the value with a "@"-character.

```
************************************************
* Program iGeoT Version 2.1     LBNL/ESD 2016 *
************************************************

Geothermal Water Chachimbiro, spring waters sampled 7/24/2001    *BATCH*
**************************************************************************

Geothermometry calculations using the flagged minerals below

Water   1     ID: Chachi-101     stwf= 0.112  cfact= 1.863   stwf iter= 0
-------------------------------------------------------------------------
Classical Geothermometers     T(C)   (for info only, reconstructed water)
---------------------------------
  Quartz  (Four&Pott82) :    226.0   (no steam loss)
  Am.Silica    (Four77) :     99.4
  Chalcedony   (Four77) :    210.9
  Na-K-Ca (Four&True73) :    220.1
  Na-K        (Gigg88) :    246.5   (Four79)   232.3
  K-Mg        (Gigg88) :    330.4
  Na-Li   (Foui&Mich81) :    449.9


---------------------------------
Multicomponent Geothermometer T(C)
---------------------------------
  T(C) cross average    : 250.6  T cross SDEV :  21.234
                                 T range      :   214.3 - 277.3
  T(C) at minimum RMED  : 250.3  minimum RMED :   0.015 T Spread : 62.9
  T(C) at minimum RMSE  : 250.8  minimum RMSE :   0.028
  T(C) at minimum SDEV  : 253.5  minimum SDEV :   0.014
  T(C) at minimum MEAN  : 250.2  minimum MEAN :   0.020
  T(C) weighted average : 251.4
  number of minerals                          :        6
  optimgeot(1) = Trmed-Tstatav                :   1.1686
  optimgeot(2) = RMED/nmina                   :   0.0025
```

Figure 3. Excerpt of restructured GeoT output showing real-valued reservoir temperature estimates.

4. PARAMETER ESTIMATION WITH iGeoT

4.1 General Concept

iGeoT automatically estimates unknown or uncertain geochemical parameters that are necessary to reconstruct the composition of deep fluids. These parameters are GeoT input variables; they include steam weight fractions (variable *stwf*) or concentration/dilution factors (variable *cfact*) for select waters, and input concentrations (variable *input-c*) for select species and waters. The parameters are estimated by maximizing the clustering (or minimizing the spread) of mineral saturation indices near zero. Various clustering measures can be selected (see Table 1), with a value of zero indicating that all saturation-index lines intersect at a single point where $\log(Q/K) = 0$.

The clustering measures are combined in an objective function, which is minimized using one of several available minimization algorithms. These algorithms can be classified as either derivative-free or derivative-based methods. Derivative-free methods make no (or only a few) assumptions about the topology of the objective function, whereas derivative-based methods require that the objective function be convex, continuous and smooth as the GeoT input parameters are varied. There is a trade-off between the generality and robustness of derivative-free, direct-search, global minimization algorithms (such as Simulated Annealing, Genetic Algorithms, and Harmony Search), and the elegance and efficiency of derivative-based, local minimization algorithms (such as the Gauss-Newton and Levenberg-Marquardt algorithms). Once the best-estimate parameter set is identified, various residual, error, and uncertainty analyses are performed, usually under the assumption of linearity and normality.

Inverse modeling theory and the detailed implementation of related methods in the iTOUGH2 simulation-optimization framework are described in *Finsterle* [2007abc]; some aspects will be illustrated in the sample problems of Section 5.

The following subsections describe the iGeoT-specific commands in the iGeoT control file, which is a separate file to be prepared if iGeoT is run in Expert Mode. No such file is needed if iGeoT is run in Automatic Mode, in which case the control file is generated internally and returned to the user for inspection and/or modification.

The iGeoT input file follows the syntax of a standard iTOUGH2 control file [*Finsterle*, 2007b], as summarized in Section 4.2.

4.2 Basic Elements of iGeoT Command Language

iGeoT is controlled by means of a high-level input language. The commands are hierarchically structured, i.e., each command has a parent command on a higher command level, and potentially one or more child commands on a lower command level. The command level is identified by the corresponding number of > markers (e.g., >>> to enter a third-level command). Each command level must be terminated by a reversed marker (e.g., <<< to quit command level three and return to level two). The position of the command level marker on a line is irrelevant.

A line without a command level marker is considered a comment and is skipped, unless it contains data requested by a previous command. Entire sections of the input file may be commented out by marking the first and last line with slash-star (/*) and star-slash (*/), respectively. All lines

---

between these two marks are not interpreted even if they contain command level markers. The number sign (#) in the first column comments out the respective line. The double-slash (//) tells iGeoT to ignore everything between the slashes and the end of the line.

On the line containing a command level marker, a command is expected which is unique to the corresponding command level and the parent command. A command can be complemented by optional keywords. Additional text present on the command line is ignored. Commands and keywords are case-insensitive. The position of the command and keywords on a command line is irrelevant. Many commands request additional numerical or alphanumeric input. This input can be provided anywhere on the command line, but must immediately preceded by a colon (:). Input may consist of one or more integers, real numbers, or strings. Input belonging to the same command can be continued on multiple lines by using the ampersand (&) character. Each line of the input file is processed word by word, the delimiter being one or more spaces. All numerical data are read in free format. Long lists of data start one line after the command line. Data lists will be read until a Fortran reading error occurs.

In general, subcommands of the same parent command can be provided in arbitrary order. A few exceptions apply; they are clearly identified when using an incorrect order.

There are three main blocks in the iGeoT control file, identified by one of the following first-level commands:

```
> PARAMETER
> OBSERVATION
> COMPUTATION
```

The first block (first-level command > PARAMETER) is used to identify those GeoT input parameters that will be subjected to parameter estimation, sensitivity analysis, or uncertainty propagation analysis. A series of subcommands ensures a unique identification of the parameter by providing its type (second-level command), and the water (and species) it is referring to (third-level command). The fourth-level commands are used to provide further information along with statistical details about the parameter.

The second block (first-level command > OBSERVATION) is used to identify the clustering measures that are to be minimized. A GeoT clustering measure is identified by the second-level command >> GeoT, its type and to which water it refers to (third-level command), as well as more detailed specifications, specifically the weight given to the criterion (fourth-level command). The calculated clustering measure is automatically compared to the theoretical optimal value of zero.

The third block (first-level command > COMPUTATION) is used for various program options and computational parameters. It deals with the choice of the minimization algorithm, convergence criteria, the numerical calculation of the Jacobian matrix, statistical parameters for the error analysis, and output options. Finally, the application mode of iGeoT (parameter estimation, sensitivity analysis, uncertainty propagation analysis) can be selected along with a number of additional features. Figure 4 shows an example of an iGeoT control file.

```
> PARAMETER

  >> GeoT                 STWF
     >>> WATER         : Chachi-101
         >>>> ANNOTATION: STWF Chachi-101
         >>>> VALUE
         >>>> RANGE      :  0.0   1.0
         >>>> DEVIATION :  0.1
         <<<<
     <<<

  >> GeoT                 CFACT
     >>> WATER         : Chachi-101
         >>>> ANNOTATION: Dilution W101
         >>>> VALUE
         >>>> PRIOR      :  0.3
         >>>> DEVIATION :  0.1
         <<<<
     <<<

  >> GeoT                 INPUT-C
     >>> SPECIES       : Al+++ Chachi-101
         >>>> ANNOTATION: Al3+ in Wat.101
         >>>> LOGARITHM
         >>>> PRIOR      : -10.0
         >>>> DEVIATION :   1.0
         <<<<
     <<<
  <<

> OBSERVATION

  >> GEOT
     >>> CLUSTER SPREAD WATER: Chachi-101
         >>>> WEIGHT: 1.0
         <<<<

     >>> CLUSTER OPTIM WATER: Chachi-101
         >>>> INDEX : 1
         >>>> WEIGHT: 1.0
         <<<<

     >>> CLUSTER OPTIM WATER: Chachi-101
         >>>> INDEX : 2
         >>>> WEIGHT: 1.0
         <<<<

     <<<
  <<

> COMPUTATION

  thermodynamic database FILE: tDB.dat

  >> CONVERGENCE criteria
     >>> stop after : 10 ITERATIONS
     <<<
  <<
```

Figure 4. Main structure of the iGeoT control file (default name *iGeoT.inp*).

4.3 iGeoT block > `PARAMETER`

The first-level command > `PARAMETER` is used to select the GeoT input parameters that may be adjusted by iGeoT to minimize the clustering measures.

The second-level command is `>> GeoT`, followed by a keyword that identifies the parameter type. The keywords are identical with the GeoT variable names (or an alternative), i.e., `STWF` (or `STEAM`) for steam weight fraction, `CFACT` (or `FACTOR`) for the concentration (or dilution) factor, `INPUT-C` (or `COMPOSITION`) for the aqueous concentration of a species, `GMOLF` (or `GASCONCENTRATION`) for gas concentration, and `LG_LOG` (or `FUGACITY`) for the logatithm of fugacity.

The third-level command for estimating steam weight fractions and concentration factors is `>>> WATER:`, followed by the water ID, which is a name up to 20 characters in length. If estimating input aqueous or gas concentrations or fugacity, the third-level command is `>>> SPECIES:`, followed by the species name (exactly as defined in the thermodynamic database file except for upper or lower case and charge notation (e.g., `Al+++`, `Al+3`, `al+++`, or `al+3` are all assumed the same) and the water ID. Species name and water ID have to be separated by at least one blank; quotes are not needed.

Various fourth-level commands can be used to further specify the parameter. For example, a parameter name can be specified using command `>>>> ANNOTATION`. Commands `>>>> VALUE` or `>>>> LOGARITHM` indicate whether the parameter itself or its logarithm (recommended for `INPUT-C`) should be estimated. It is advisable to also specify an admissible parameter `>>>> RANGE` as well as a standard `>>>> DEVIATION` to condition the inversion of the initial `>>>> GUESS`. The usage of these and additional fourth-level commands in described in *Finsterle* [2007b]. See Figure 4 for an example.

4.4 iGeoT block > `OBSERVATION`

Commands below the first-level command > `OBSERVATION` and second-level command `>> GeoT` are used to select the GeoT clustering measures. Each of these measures assumes a value of zero for a perfect, consistent identification of reservoir temperature. The select GeoT input parameters (see Section 4.3) are estimated by minimizing an objective function that consists of the sum of the squared, weighted selected clustering measures. These clustering measures are shown in Table 1. Note that objective functions other than weighted least squares can be chosen by the user when iGeoT is run in expert mode.

Examples of the iGeoT `>> OBSERVATION` block can be found in Section 5.

Table 1: Clustering measures

Cluster ID	Keyword	Statistics	Explanation	Default[d] σ_p
1.1[c]	SATURATION[a]	MEDIAN	Median of SI at minimum of median of SI	$1/\sqrt{n_m}$
1.2[c]	SATURATION	MEAN	Mean of SI at minimum of median of SI	$1/\sqrt{n_m}$
1.3[c]	SATURATION	SIGMA	Standard deviation of SI at minimum of median of SI	1
1.4[c]	SATURATION	RMSE	RMSE of SI at minimum of median of SI	1
2.1[c]	SPREAD	MEAN	Temperature spread	ΔT
2.2[c]	SPREAD	SIGMA	Standard deviation of crossing temperature	$\Delta T/6$
3.1	GLOBAL[b]	ESTI-MATED	Standard deviation of average estimated temperature	$\Delta T/\sqrt{n_w}$
3.2	GLOBAL[b]	OTHER	Standard deviation of temperature of $T_{stat,ave} = (T_{min,mean} + T_{min,sigma} + T_{min,rmse})\,/\,3$	$\Delta T/\sqrt{3 \cdot n_w}$
3.3	GLOBAL[b]	RANGE	Standard deviation of temperature range	$\Delta T/\sqrt{n_w}$
3.4	GLOBAL[b]	CROSS	Standard deviation of crossing temperature	$\Delta T/\sqrt{n_w}$
4.1	OPTIMization		$T_{min,med}$ - $T_{stat,ave}$	$\Delta T/\sqrt{1.65 \cdot n_m}$

[a] : Refers to saturation index $SI = \log (Q/K)$

[b] : Only if multiple waters are analyzed

[c] : Provide water name on command line using keyword, i.e., WATER: *water_name*

[d] : Default standard deviations assigned to clustering measure if iGeoT is run in automatic mode (see Section 4.5); n_m is number of minerals; n_w is number of waters; $\Delta T = T_{end}$ - T_{start} is the user-specified temperature range evaluated by GeoT

4.5 iGeoT Automatic Mode

To guide the inversion, the user has access to all features and control parameters implemented in iTOUGH2 [*Finsterle*, 2007b], including selection of (1) the application mode (forward run, sensitivity analysis, parameter estimation, uncertainty analysis), (2) the minimization algorithm (derivative-based or sampling-based, local or global), (3) weighting coefficients assigned to individual clustering measures and/or prior information about the parameters to be estimated, (4) admissible parameter ranges and parameter transformations, and (5) computational parameters and convergence criteria. This flexibility is useful and needed as iTOUGH2 is applicable to a wide variety of optimization problems.

However, the purpose of iGeoT is to solve a specific inverse problem, i.e., an application in which a limited number of pre-defined parameters are estimated by minimizing a limited number of clustering measures. This makes it possible to define a set of control parameters that likely yields a robust solution for many iGeoT inverse problems. Setting up an iGeoT optimization run can thus be largely automated; this is referred to as the *iGeoT Automatic Mode*. The user is still given the

possibility to interfere and customize the inversion should the automatic approach fail; this is referred to as the *iGeoT Expert Mode*.

To run iGeoT in automatic mode, the user does not need to be familiar with any of the iTOUGH2 control parameters or its input format; all the user needs to do is identify in a standard GeoT input file, which of its parameters shall be estimated. This is accomplished by simply labeling the value in the GeoT input with the character "@", either preceding or following the numerical value of the parameter to be estimated (without a space between "@" and the numbers). **Figure 5** shows an excerpt of a GeoT input file. The values of the steam weight fraction, concentration factor, and the input molality of two dissolved species are labeled with the "@" character as parameters to be estimated by iGeoT. The value given in the GeoT input file is used as the initial guess of the respective parameter. Moreover, iGeoT automatically performs appropriate parameter transformations for a given parameter type, sets bounding values, and selects suitable clustering measures and their relative weights (see last column of Table 1). The Levenberg-Marquardt minimization algorithm and reasonable convergence criteria are invoked to solve the inverse problem. All these control parameters are written in standard iGeoT format to a file with the extension *.iGeoT*; this file is made available to the user after iGeoT is run in automatic mode.

To run iGeoT in automatic mode, the user needs to provide the GeoT input file (with the uncertain parameters labeled as shown in **Figure 5**) along with a dummy iGeoT input file that contains the keyword `AUTOMATIC` in the first line (see also Section 3.2 for details about specifying the thermodynamic database). The inversion results are reported in a standard iGeoT output file.

When estimating input parameters with iGeoT (in automatic or expert mode), it is highly recommended to work with a fixed number of minerals, thus to set the *min_elim* input parameter equal to the exact number of specified minerals (i.e., no mineral elimination) and not to use the *include_minerals* or *skip_minerals* options. Doing otherwise may result in highly discontinuous objective functions as different minerals may be dynamically picked up during the optimization and thus increase the likelihood of optimization convergence to a false minimum.

```
# ID                      tc      keepic      stwf        cfact
Water1                    25.0      0         @0.04       @2.00


#name    icon   guess(molal)     input(mol)
H+        1      1.00E-08       -0.46142E-03
H2O       1      1.00            0.10000E+01
SiO2(aq)  1      1.00E-06        0.30933E-02
Na+       1      1.00E-06        0.10211E-01@
K+        1      1.00E-06        0.80995E-03
Ca++      1      1.00E-06        0.41806E-04
Mg++      1      1.00E-06        0.21418E-06
H3BO3     1      1.00E-06        0.30973E-03
HCO3-     1      1.00E-06        0.20620E-02@
SO4--     1      1.00E-06        0.23255E-02
Cl-       1      1.00E-06        0.32846E-02
F-        1      1.00E-06        0.67470E-03
Al+++     1      1.00E-10        0.97371E-05
'*'
```

Figure 5. iGeoT Automatic Mode: Excerpt of a GeoT input file showing the labeling of the parameter to be estimated.

5. EXAMPLE

The example in this section is tutorial. Its purpose is to demonstrate the usage of iGeoT features and is not of scientific value.

In this example [*Sycher et al.*, 2016b] we consider a synthetic geothermal fluid in a deep reservoir that is equilibrated at 250 °C with a mineral assemblage consisting of quartz, calcite, anhydrite, fluorite, clchlore, heulandi, microcli, and albit-lo at a CO_2 fugacity (~pressure) of 5 bar. From this "mother" fluid, two derived synthetic waters were numerically created:

- Derived water 1 (*no-react-degas*), obtained by cooling the mother fluid to 50 °C and degassing it to a log(PCO_2) value of -3 at 50 °C, followed by dilution by a factor of 2, and
- Derived water 2 (*no-react-degas2*), obtained by cooling the mother fluid to 25 °C and degassing it a log(PCO_2) value of -3.5 at 25 °C, then diluting it by a factor of 3.

These two synthetic fluids were then used with iGeoT to reconstruct the composition of the deep "mother" fluid and calculate its original temperature.

Below, we discuss how to run iGeoT using these two derived waters as an example, first without parameter estimation (Section 5.1), then with estimation of the dilution factor and amount of CO_2 loss to reconstruct the deep fluid in AUTOMATIC mode (Section 5.2), then in EXPERT mode (Section 5.3). A partial (incomplete) input file for this problem is shown below (**Figure 6**), to illustrate the input of these two water compositions.

We repeat here the recommendation to set the *min_elim* input parameter equal to the exact number of specified minerals when estimating input parameters with iGeoT in automatic or expert mode. Doing otherwise, or using the *include_minerals* or *skip_minerals* options, will increase the likelihood of optimization convergence to a false minimum. The use of these options and mineral elimination with iGeoT is still appropriate for forward runs, i.e., when estimating reservoir temperature without optimization of other input parameters.

```
######################################################################
# Program geoT annotated example input file                         #
######################################################################

# All blank lines or those starting with # are not read on input
# All entries must appear in the order shown (in free format)

# Always use "#" as first character of comment lines
# Blank lines are ignored
# Strings can be in quotes or not, but quotes are needed if string contains
# blanks except for the title

# Title comes first (one record below)
Artificial geothermal water at 250 C, 3 bar CO2  (Equilibrate SV Phipps-2 water)
*BATCH*

# thermodynamic database
tk-slt.h06_jun16.dat

# PRIMARY AQUEOUS SPECIES - always end the list with a star (in quotes or not)
H+
H2O
SiO2(aq)
Na+
K+
Ca++
Mg++
H3BO3
HCO3-
SO4--
Cl-
F-
Al+++
'*'

# WATER COMPOSITIONS
# ID:    40-character water ID
# tc:    initial speciation temperature in (C)
# keepic: unused
#
# stwf:  steam (total gases) weight fraction in total discharge (for gas
#        corrections; if zero no gas is added)
# cfact: concentration factor  (1=no concentration, > 1 for concentration,
#        < 1 for dilution) (multiplies input concentrations)
# soldens (V1.5 and above):  solution density for concentration unit conversions,
#                            in g/cc = kg/l - defaults to 1
#
# pmix:  mixing proportions for each mixing endmembers
#        (0 or blank =none, 2 = 2:1 mixing, etc.),
#        enter one pmix per mixing waters
# name:  name of primary species (at minimum H+ and H2O) - any order
# icon: 1 input concentration is total moles (for water total kg, generally 1kg)
#       2 constrained by equilibrium with specified mineral at given log(Q/K),
#         but only at initialization temperature tc
#       3 input concentration is activity (use for pH) (only at initialization
#         temperature tc)
#       4 input concentration will be adjusted for charge balance (at all
#         temperatures) (if the species charge sign is the same as the charge
#         imbalance, will not converge - pick a species with opposite charge)
```

```
#        5 constrained by equilibrium with specified mineral at given log(Q/K),
#           but only at T=tstart and above (to avoid convergence problems at low T)
#        6 constrained by equilibrium with specified mineral at given log(Q/K) at
#           all temperatures
#        7 input concentration is activity (e.g., use for pH) remains fixed at all
#           temperatures

# trial_c: initial guess for NR iterations (generally use same as input
#          molalities)
#            (affects initial speciation convergence, but does not affect results)
# input_c:  moles of dissolved species and kg of water
#          V1.5 and above: other concentrations units can be entered if followed
#          by the following strings
#          (note, case insensitive, quotes are required if units contains a "/")
#                ppm  ppb mgl ugl molar mmolar umolar molal mmolal umolal 'mg/L'
#                'ug/L'  'mmol/kg'  'umol/kg'  'mmol/L'  'umol/L'
#                By default, mass units are converted using the molecular weight
#                of the primary species, unless the element is specified as
#                follows, e.g.:  200 ppm as Si   (the "as" is required)
#
# name_eq: name of mineral fixing the concentration of that species
#          (enabled when icon=2)
# cfact:  desired saturation index of constraining mineral (enabled when icon=2)


# ID                      tc      keepic        stwf          cfact
no-react-degas          25.0     0            @.01          @1.1

#name  icon   trial_c(molal)  input_c (mol)   name_eq  logqk
H+        1    1.00E-08       -0.46142E-03
H2O       1    1.00            0.10000E+01
SiO2(aq) 1    1.00E-06        0.30933E-02
Na+       1    1.00E-06        0.10211E-01
K+        1    1.00E-06        0.80995E-03
Ca++      1    1.00E-06        0.41806E-04
Mg++      1    1.00E-06        0.21418E-06
H3BO3     1    1.00E-06        0.30973E-03
HCO3-     1    1.00E-06        0.20620E-02
SO4--     1    1.00E-06        0.23255E-02
Cl-       1    1.00E-06        0.32846E-02
F-        1    1.00E-06        0.67470E-03
Al+++     1    1.00E-10        0.97371E-05
'*'

# ID                      tc      keepic        stwf          cfact
no-react-degas2         25.0     0            @.01          @1.1

#name  icon  guess(molal)    input(mol)      constr.  sat.
H+        1    1.00E-08       -0.28431E-03
H2O       1    1.00            0.10000E+01
SiO2(aq) 1    1.00E-06        0.20622E-02
Na+       1    1.00E-06        0.68070E-02
K+        1    1.00E-06        0.53997E-03
Ca++      1    1.00E-06        0.27871E-04
Mg++      1    1.00E-06        0.14279E-06
H3BO3     1    1.00E-06        0.20649E-03
HCO3-     1    1.00E-06        0.13980E-02
SO4--     1    1.00E-06        0.15503E-02
Cl-       1    1.00E-06        0.21897E-02
F-        1    1.00E-06        0.44980E-03
Al+++     1    1.00E-10        0.64914E-05
'*'
```

```
#repeat as many waters as desired starting with the ID record
#always end with this record:
end_waters

# !!! The last part below is in beta-testing
############################################

#OPTIONAL MIXING END-MEMBERS
#flag (Yes/no)   If no, or not there, no further records are read
#If yes, enter mixing end-members that will be "de-mixed" from the other waters
no
```

Figure 6. GeoT input file *geot.inp*.

5.1 Running iGeoT in Forward Mode (Without Parameter Estimation)

For a run without parameter estimation, the "@" characters next to the *stwf* and *cfact* input values in Figure 6 can be removed, thus the input file is identical in format to a regular GeoT input file.

The simplest way to run iGeoT without parameter estimation is to execute the code by typing the name of the executable at the command prompt, for example:

iGeoT1.0-2.1-PC64 (Windows)

or

iGeoT1.0-2.1-OSX10.9 (Mac)

In this case, iGeoT prompts the user for the name of the input file (by default *geot.inp*) then for the name of the file with inversion parameters (by default *igeot.inp*), which must be present in the current folder, but is left blank (dummy file) since no parameter estimation is desired.

Alternatively, one could use the provided iGeoT script (only for Mac/Linux):

geot geot.inp

and provide the name of the database file and GeoT input file on the command line. Note that in this case the thermodynamic database file needs to be provided on the command line using the argument −fi *filename*. The file needs to be in the working directory.

An example GeoT output file is shown in **Figure 7**. Note that the estimated reservoir temperature is different from the true value of 250 °C, because the steam weight fractions (stwf) and dilution factors (cfact) for the two waters are inaccurate, leading to imperfect clustering of the saturation lines.

It is the purpose of iGeoT to obtain estimates of stwf and cfact such that the clustering is maximized, leading to a better estimate of reservoir temperature using multicomponent geothermometry. This is demonstrated in Section 5.2.

```
************************************************
* Program iGeoT Version 2.1     LBNL/ESD 2016 *
************************************************


Artificial geothermal water at 250 C
******************************************************************************


Geothermometry calculations using the flagged minerals below

Water   1    ID: no-react-degas                         stwf = 0.000 cfact = 1.000  stwf iter = 0
--------------------------------------------------------------------------------------
Classical Geothermometers      T(C)  (for info only, reconstructed water, zero if no data)
--------------------------------
  Quartz  (Four&Pott82) :    175.6  (no steam loss)
  Am.Silica    (Four77) :     51.6
  Chalcedony   (Four77) :    153.2
  Na-K-Ca (Four&True73) :    229.8
  Na-K        (Gigg88) :    257.4  (Four79)  244.1
  K-Mg        (Gigg88) :    232.9
  Na-Li   (Foui&Mich81) :      0.0


--------------------------------
Multicomponent Geothermometer T(C)
--------------------------------
  T(C) cross average    :    148.7  T cross SDEV :  43.054        T range  :   100.0 - 201.6
  T(C) at minimum RMED  :    189.8  minimum RMED :   0.173        T spread :   101.6
  T(C) at minimum RMSE  :    194.1  minimum RMSE :   0.938
  T(C) at minimum SDEV  :    100.0  minimum SDEV :   0.638
  T(C) at minimum MEAN  :    191.3  minimum MEAN :   0.601
  T(C) weighted average :    176.5  number of minerals selected for T estimation :  8
                                    optimgeot(1) = Trmed-Tstatav                 : 28.0033
                                    optimgeot(2) = RMED/nmina                    :  0.0216
```

```
Temperature (C) --->      100.00   110.00   120.00   130.00   140.00   150.00   160.00   170.00 >>>
Gas sat. P(bar) --->        1.03     1.45     2.01     2.74     3.67     4.83     6.27     8.04
Iterations                    15        5        5        5        5        5        5        4

 pH                         7.94     7.90     7.86     7.83     7.81     7.79     7.77     7.76


 RMED                       1.10     0.96     0.83     0.70     0.58     0.47     0.36     0.25
 RMSE                       1.26     1.20     1.14     1.09     1.05     1.01     0.98     0.96
 SDEV                       0.64     0.65     0.67     0.69     0.71     0.73     0.74     0.76
 MEAN                       1.11     1.03     0.96     0.88     0.81     0.74     0.69     0.64

              Scaled saturation indices:  * (or **) if mineral selected for statistics, ** if
microcli        **   1.07     0.92     0.79     0.66     0.53     0.42     0.31     0.20
quartz          **   0.46     0.39     0.31     0.24     0.18     0.12     0.06     0.01
albit-lo        **   0.72     0.61     0.50     0.40     0.30     0.21     0.13     0.05
heulandi        **   1.14     1.00     0.87     0.75     0.63     0.52     0.41     0.30
calcite         *   -0.32    -0.25    -0.19    -0.12    -0.06     0.00     0.06     0.12
fluorite        *   -1.23    -1.22    -1.20    -1.17    -1.15    -1.12    -1.09    -1.06
anhydrit        *   -2.24    -2.10    -1.96    -1.83    -1.69    -1.56    -1.44    -1.31
clchlore        *    1.71     1.78     1.84     1.89     1.95     2.00     2.04     2.09

              Mole fractions at saturation
h2o(g)             0.995E+00 0.996E+00 0.996E+00 0.996E+00 0.996E+00 0.997E+00 0.997E+00 0.997E+00
co2(g)             0.464E-02 0.432E-02 0.404E-02 0.380E-02 0.357E-02 0.336E-02 0.315E-02 0.296E-02

              Partial pressures (bar)
h2o(g)             0.102E+01 0.145E+01 0.201E+01 0.273E+01 0.365E+01 0.482E+01 0.625E+01 0.801E+01
co2(g)             0.476E-02 0.627E-02 0.814E-02 0.104E-01 0.131E-01 0.162E-01 0.198E-01 0.238E-01



Water   2    ID: no-react-degas2                          stwf = 0.000 cfact = 1.000  stwf iter = 0
----------------------------------------------------------------------------------------------------
Classical Geothermometers    T(C)  (for info only, reconstructed water, zero if no data)
----------------------------------
  Quartz  (Four&Pott82) :    149.7  (no steam loss)
  Am.Silica   (Four77) :     28.1
```

```
  Chalcedony    (Four77) :      124.2
  Na-K-Ca (Four&True73) :      225.4
  Na-K        (Gigg88) :      257.4   (Four79)   244.1
  K-Mg        (Gigg88) :      222.8
  Na-Li   (Foui&Mich81) :        0.0


---------------------------------
Multicomponent Geothermometer T(C)
---------------------------------
  T(C) cross average    :      141.1   T cross SDEV :  39.246          T range  :    100.0 - 203.4
  T(C) at minimum RMED  :      162.3   minimum RMED :   0.197          T spread :    103.4
  T(C) at minimum RMSE  :      200.6   minimum RMSE :   0.896
  T(C) at minimum SDEV  :      235.1   minimum SDEV :   0.550
  T(C) at minimum MEAN  :      177.6   minimum MEAN :   0.650
  T(C) weighted average :      183.0   number of minerals selected for T estimation :  8
                                       optimgeot(1) = Trmed-Tstatav                  : 42.1096
                                       optimgeot(2) = RMED/nmina                     :  0.0247


Temperature (C) --->     100.00    110.00    120.00    130.00    140.00    150.00    160.00    170.00
Gas sat. P(bar) --->       1.02      1.45      2.01      2.74      3.67      4.83      6.27      8.03
Iterations                   24         5         5         5         5         5         5         4

 pH                        7.90      7.86      7.82      7.78      7.76      7.73      7.71      7.70


 RMED                      0.85      0.70      0.57      0.47      0.38      0.30      0.21      0.21
 RMSE                      1.25      1.18      1.12      1.07      1.03      0.99      0.96      0.93
 SDEV                      0.72      0.73      0.74      0.75      0.76      0.74      0.73      0.71
 MEAN                      1.05      0.97      0.89      0.82      0.74      0.70      0.67      0.65


              Scaled saturation indices:  * (or **) if mineral selected for statistics, ** if
 microcli          **    0.79      0.64      0.51      0.38      0.26      0.14      0.03     -0.07
 quartz            **    0.29      0.22      0.14      0.08      0.01     -0.05     -0.11     -0.16
 heulandi          **    0.90      0.77      0.64      0.52      0.40      0.29      0.18      0.08
 albit-lo          **    0.44      0.33      0.22      0.12      0.03     -0.06     -0.15     -0.23
 calcite           *    -0.63     -0.56     -0.49     -0.43     -0.36     -0.30     -0.24     -0.18
 clchlore          *     1.18      1.24      1.30      1.35      1.40      1.44      1.49      1.53
 fluorite          *    -1.68     -1.65     -1.63     -1.60     -1.57     -1.54     -1.50     -1.47
 anhydrit          *    -2.48     -2.34     -2.19     -2.05     -1.91     -1.78     -1.64     -1.51
```

```
                      Mole fractions at saturation
h2o(g)                0.997E+00 0.997E+00 0.997E+00 0.997E+00 0.997E+00 0.997E+00 0.998E+00 0.998E+00
co2(g)                0.349E-02 0.328E-02 0.310E-02 0.293E-02 0.277E-02 0.262E-02 0.247E-02 0.233E-02


                      Partial pressures (bar)
h2o(g)                0.102E+01 0.145E+01 0.201E+01 0.273E+01 0.365E+01 0.482E+01 0.625E+01 0.801E+01
co2(g)                0.357E-02 0.475E-02 0.623E-02 0.802E-02 0.102E-01 0.127E-01 0.155E-01 0.187E-01




 *******************************************************
 Global optimization data (to use with multiple waters):
    Average estimated T =   176.057  stdev =  19.434224
    Average T other stat=   183.110  stdev =  30.143088
    Average of T range  =   144.899  stdev =   5.368159
    Average T spread    =   102.520  stdev =   1.254094
```

Figure 7. GeoT output file *geot.out*.

5.2 Estimating Parameters using iGeoT in Automatic Mode

Using the previous example, we now estimate four uncertain parameters (i.e., the steam weight fractions and dilution factors of each of the two waters) by minimizing the clustering measures with iGeoT in automatic mode. The GeoT input file (*geot.inp* by default) is similar to that shown in **Figure 6**. Note how the four parameters of interest are identified by the labeling character "@". In this case, the input values for these parameters are taken as initial guesses for the optimization. The closer these values are to their "true" values, the more chance of a successful optimization. To ensure that the optimization converges to a true minima, it is recommended that more than one iGeoT run be conducted, each time specifying different initial values for the parameters that are estimated, to check that the solutions for these runs do not vary significantly.

The input file with optimization instructions (*igeot.inp* by default) is shown in **Figure 8**. Note that the thermodynamic database file *tk-slt.h06_jun16.dat* also always needs to be present in the working folder.

```
AUTOMATIC
thermodynamic database FILE: tk-slt.h06_jun16.dat
```

Figure 8. iGeoT input file *igeot.inp* for automatic.

This test problem is run under Linux using the following command line

```
igeot igeot.inp geot.inp
```

or by simply typing the name of the executable under Windows and typing <return> when prompted for input file names, which results in the default file names being used.

iGeoT automatically generates the iGeoT input file shown in **Figure 9** and stores it under the name geot.*iGeoT*. It contains the `> PARAMETER` block wit the four parameters to be estimated. The `> OBSERVATION` block shows the automatically selected clustering measures, which consist of two sets, one for each water. The cluster measures included are measures 1.1 – 1.4, 2.1, 2.2, and 4.1 in Table 1. In addition, since two waters are present, the global clustering measures (measures 3.1 – 3.4; see Table 1) are also included. A maximum of 16 Levenberg-Marquardt iterations are performed.

After internally generating file *geot.iGeoT*, the inversion is initiated without the need for user interference. The results of the inversion are output in file *igeot.out* (see **Figure 10**). A short discussion of the main blocks in the iGeoT output file *igeot.out* is provided here; more details can be found in the documentation of the iTOUGH2 simulation-optimization code.

The first block (labeled "`INPUT`") first reports the parameters to be estimated by iGeoT, with their names, initial guesses, standard deviations (used to weigh prior information), and admissible parameter ranges. This is followed by the list of clustering measures and their respective standard deviations. Recall that the target value for each of these measures is zero. Computational parameters related to the algorithm used to minimize the objective function and information about the computer system is also provided.

The second block (labeled "`OUTPUT`") contains information about the inversion process and its results. A log of the search path taken in the *n*-dimensional parameter space is provided first, followed by block labeled "`SENSITIVITY ANALYSIS`", which is a printout of the scaled

sensitivity coefficients (i.e., the partial derivative of each clustering measure with respect to the parameters to be estimated) and some composite sensitivity measures.

The block labeled "`ERROR ANALYSIS`" shows the covariance matrix of the estimated parameters, which holds the error variances on its diagonal. Correlation coefficients, marginal and conditional standard deviations, and measures of overall parameter independence are also provided.

The block labeled "`RESIDUAL ANALYSIS`" lists the computed clustering measure obtained with the optimum parameter set. Summary statistics about the final residuals are also provided.

The final block summarizes the results, i.e., the best estimate parameter values, their (marginal) estimation uncertainty, and composite sensitivity measures.

The GeoT output file obtained with the optimized parameter set is named *geot.out* (see **Figure 11**). It shows that a reservoir temperature of 250 °C — i.e., the "true" temperature — is obtained after estimating the unknown (or uncertain) steam weight fractions and water dilution factors of the two water samples available for multicomponent geothermometry.

```
File *samGEOT1.iGeoT* was automatically generated by iGeoT
from GeoT input file.

GeoT thermodynamic database FILE: tk-slt.h06_jan14.dat

> PARAMETER

  >> GeoT                STWF
     >>> WATER          : no-react-degas
         >>>> VALUE
         >>>> PRIOR     :  0.100000E-01
         >>>> DEVIATION :  0.100000E+05
         <<<<
     <<<

  >> GeoT                CFACT
     >>> WATER          : no-react-degas
         >>>> VALUE
         >>>> PRIOR     :  0.100000E+01
         >>>> DEVIATION :  0.100000E+05
         <<<<
     <<<

  >> GeoT                STWF
     >>> WATER          : no-react-degas2
         >>>> VALUE
         >>>> PRIOR     :  0.100000E-01
         >>>> DEVIATION :  0.100000E+05
         <<<<
     <<<

  >> GeoT                CFACT
     >>> WATER          : no-react-degas2
         >>>> VALUE
         >>>> PRIOR     :  0.110000E+01
         >>>> DEVIATION :  0.100000E+05
         <<<<
     <<<
  <<

> OBSERVATION

  >> GeoT
     >>> CLUSTER 1.1 - SATURATION MEDIAN WATER: no-react-degas
         >>>> WEIGHT: 2.82843
         <<<<

     >>> CLUSTER 1.2 - SATURATION MEAN   WATER: no-react-degas
         >>>> WEIGHT: 2.82843
         <<<<

     >>> CLUSTER 1.3 - SATURATION SIGMA  WATER: no-react-degas
         >>>> WEIGHT: 1.00000
         <<<<
```

```
   >>> CLUSTER 1.4 - SATURATION RMSE   WATER: no-react-degas
       >>>> WEIGHT: 1.00000
       <<<<

   >>> CLUSTER 2.1 - SPREAD MEAN       WATER: no-react-degas
       >>>> WEIGHT: 0.00500
       <<<<

   >>> CLUSTER 2.2 - SPREAD SIGMA      WATER: no-react-degas
       >>>> WEIGHT: 0.03000
       <<<<

   >>> CLUSTER 4.1 - OPTIMIZATION      WATER: no-react-degas
       >>>> WEIGHT: 0.01000
       <<<<

   >>> CLUSTER 1.1 - SATURATION MEDIAN WATER: no-react-degas2
       >>>> WEIGHT: 2.82843
       <<<<

   >>> CLUSTER 1.2 - SATURATION MEAN   WATER: no-react-degas2
       >>>> WEIGHT: 2.82843
       <<<<

   >>> CLUSTER 1.3 - SATURATION SIGMA  WATER: no-react-degas2
       >>>> WEIGHT: 1.00000
       <<<<

   >>> CLUSTER 1.4 - SATURATION RMSE   WATER: no-react-degas2
       >>>> WEIGHT: 1.00000
       <<<<

   >>> CLUSTER 2.1 - SPREAD MEAN       WATER: no-react-degas2
       >>>> WEIGHT: 0.00500
       <<<<

   >>> CLUSTER 2.2 - SPREAD SIGMA      WATER: no-react-degas2
       >>>> WEIGHT: 0.03000
       <<<<

   >>> CLUSTER 4.1 - OPTIMIZATION      WATER: no-react-degas2
       >>>> WEIGHT: 0.01000
       <<<<


 Global clustering measures; number of waters:  2

   >>> CLUSTER 3.1 - GLOBAL ESTIMATED
       >>>> WEIGHT: 0.00500
       <<<<

   >>> CLUSTER 3.2 - GLOBAL OTHER
       >>>> WEIGHT: 0.00866
       <<<<

   >>> CLUSTER 3.3 - GLOBAL RANGE
```

```
        >>>> WEIGHT: 0.00500
        <<<<

    >>> CLUSTER 3.4 - GLOBAL CROSS
        >>>> WEIGHT: 0.00825
        <<<<
    <<<
  <<

> COMPUTATION

  >> STOP
    >>> ITERATIONS:  16
    <<<

  >> JACOBIAN
#     >>> CENTERED
    >>> PERTURB: 0.01
    <<<

  >> OUTPUT
#     >>> RESIDUAL
    <<<
  <<
<
```

Figure 9. Automatically generated iGeoT file *iGeoT.inp*.

```
                    @@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@
                    @                                  @
                    @   @   @@@  @@@@  @@   @@@@@  @
                    @       @    @   @ @ @     @    @
                    @   @ @ @@   @@@   @ @   @    @
                    @   @ @ @ @  @     @ @   @    @
                    @   @   @@@  @@@@  @@    @    @
                    @                                  @
                    @@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@

            iTOUGH2 V6.9 (JUNE, 2016) FOR LINUX, N. SPYCHER AND S. FINSTERLE
             COPYRIGHT (C) 2014, THE REGENTS OF THE UNIVERSITY OF CALIFORNIA
                   THROUGH LAWRENCE BERKELEY NATIONAL LABORATORY
                            ALL RIGHTS RESERVED


=====================================================================================================
                        >>>>>>>>>>>> 27-Nov-15  14:34 <<<<<<<<<<<<
=====================================================================================================
iGEOT INPUT FILE            :   samGEOT1i
GEOT INPUT FILE             :   samGEOT1
WORKING DIRECTORY           :   /Users/SAFinsterle/itough2/Samples/sampleGEOT
TEMPORARY DIRECTORY         :   /Users/SAFinsterle/it2_64584
=====================================================================================================

--- Line    2 Start reading from include file "samGEOT1.iGeoT"; line counter reset to 0.

--- Line   164 ignored.

--- Line   168 ignored.


*****************************************************************************************************
                                           INPUT
*****************************************************************************************************


PARAMETERS
==========
-----------------------------------------------------------------------------------------------------
 # ANNOTATION         PARAMETER TYPE WATERS PRIOR INFO. INIT. GUESS  STD. DEV. LOWER BND UPPER BND MAX. STEP   INDEX
-----------------------------------------------------------------------------------------------------
 1 STWF no-react-d GeoT STWF       no-re   4.439E-02  4.4396E-02  1.000E+04  UNBOUNDED UNBOUNDED   UNLIMITED    1
 2 CFACT no-react- GeoT CFACT      no-re   2.070E+00  2.0709E+00  1.000E+04  UNBOUNDED UNBOUNDED   UNLIMITED    2
 3 STWF no-react-d GeoT STWF       no-re   3.698E-02  3.6981E-02  1.000E+04  UNBOUNDED UNBOUNDED   UNLIMITED    1
 4 CFACT no-react- GeoT CFACT      no-re   4.991E+00  4.9916E+00  1.000E+04  UNBOUNDED UNBOUNDED   UNLIMITED    2
-----------------------------------------------------------------------------------------------------
```

```
------------------------------------------------------------------------------------
 ADJUSTABLE PARAMETER = TRANSFORMED MODEL INPUT PARAMETER (MIP)
------------------------------------------------------------------------------------
 1  STWF no-react-d  =       MIP
 2  CFACT no-react-  =       MIP
 3  STWF no-react-d  =       MIP
 4  CFACT no-react-  =       MIP
------------------------------------------------------------------------------------


OBSERVATIONS
============


------------------------------------------------------------------------------------
SET ANNOTATION      CLUSTERING MEASURE              WATER     STD. DEV. LOG(V/M/S)      #DATA #CALI FACTOR IOBS
------------------------------------------------------------------------------------
 1 CLUSTER 1.1    SATURATION   MEDIAN       no-react-degas  3.53553E-01    VALUE  DATA=ZERO  1 1.00E+00   1
 2 CLUSTER 1.2    SATURATION   MEAN         no-react-degas  3.53553E-01    VALUE  DATA=ZERO  1 1.00E+00   1
 3 CLUSTER 1.3    SATURATION   SIGMA        no-react-degas  1.00000E+00    VALUE  DATA=ZERO  1 1.00E+00   1
 4 CLUSTER 1.4    SATURATION   RMSE         no-react-degas  1.00000E+00    VALUE  DATA=ZERO  1 1.00E+00   1
 5 CLUSTER 2.1    SPREAD       MEAN         no-react-degas  2.00000E+02    VALUE  DATA=ZERO  1 1.00E+00   1
 6 CLUSTER 2.2    SPREAD       SIGMA        no-react-degas  3.33333E+01    VALUE  DATA=ZERO  1 1.00E+00   1
 7 CLUSTER 4.1    OPTIM        MEASURE-1    no-react-degas  1.00000E+02    VALUE  DATA=ZERO  1 1.00E+00   1
 8 CLUSTER 1.1    SATURATION   MEDIAN       no-react-degas2 3.53553E-01    VALUE  DATA=ZERO  1 1.00E+00   1
 9 CLUSTER 1.2    SATURATION   MEAN         no-react-degas2 3.53553E-01    VALUE  DATA=ZERO  1 1.00E+00   1
10 CLUSTER 1.3    SATURATION   SIGMA        no-react-degas2 1.00000E+00    VALUE  DATA=ZERO  1 1.00E+00   1
11 CLUSTER 1.4    SATURATION   RMSE         no-react-degas2 1.00000E+00    VALUE  DATA=ZERO  1 1.00E+00   1
12 CLUSTER 2.1    SPREAD       MEAN         no-react-degas2 2.00000E+02    VALUE  DATA=ZERO  1 1.00E+00   1
13 CLUSTER 2.2    SPREAD       SIGMA        no-react-degas2 3.33333E+01    VALUE  DATA=ZERO  1 1.00E+00   1
14 CLUSTER 4.1    OPTIM        MEASURE-1    no-react-degas2 1.00000E+02    VALUE  DATA=ZERO  1 1.00E+00   1
15 CLUSTER 3.1    GLOBAL       ESTIMATED            GLOBAL  2.00000E+02    VALUE  DATA=ZERO  1 1.00E+00   1
16 CLUSTER 3.2    GLOBAL       OTHER                GLOBAL  1.15473E+02    VALUE  DATA=ZERO  1 1.00E+00   1
17 CLUSTER 3.3    GLOBAL       RANGE                GLOBAL  2.00000E+02    VALUE  DATA=ZERO  1 1.00E+00   1
18 CLUSTER 3.4    GLOBAL       CROSS                GLOBAL  1.21212E+02    VALUE  DATA=ZERO  1 1.00E+00   1
------------------------------------------------------------------------------------


--------------------------------------------------
Number of datasets                  :   18
Number of calibration times         :    1
Number of calibration points        :   18
Number of predictions               :    0
Number of dummy observations        :    0
Number of specified parameters      :    4
Number of TOUGH-related parameters  :    0
```

```
Number of TOUGH-independent parameters:    4
Number of inactive parameters         :    0
Number of tied parameters             :    0
Number of adjustable parameters   (n) :    4
Number of superparameters (max.)      :    0
Number of parameters with prior info. :         4
Number of regularization terms        :         0
Number of GEOT CLUSTERING             :        18
                                         -----
Total number of observations      (m) :        22
                                         =====
Degree of freedom              (m-n) :   18
----------------------------------------------------


COMPUTATIONAL PARAMETERS
========================

Algorithm or application mode               :        Levenberg-Marquardt
Maximum number of iTOUGH2 iterations        :                         16
Maximum number of calls to (unknown)        :                       9999
Maximum number of uphill steps              :                         10
Maximum size of scaled parameter step       :                  unlimited
Initial Levenberg parameter                 :                   1.00E+00
Marquardt parameter                         :                  -1.00E+01
Finite difference quotient for Jacobian     :                    forward
Diagonal of Tikhonov matrix                 :    Diagonal of normal matrix
Automatic FD update of Jacobian             :                          0
Skip iterations with FD update of Jacobian  :                          0
Broyden rank-one update of Jacobian         :                          0
Increment factor for computing derivatives  :                   1.00E-02
Simple parameter bounds enforced by         :        Hard parameter bounds
Variance for error analysis                 :                a posteriori
Format of plotfile                          :                    Tecplot
Objective Function                          :              Least-Squares


COMPUTER SYSTEM
===============

Machine type                      : Linux
UNIX script file name             : /Users/SAFinsterle/bin/itough2
UNIX command line arguments       : samGEOT1i samGEOT1 geot
Host name                         : finsterle
User name                         : SAFinsterle
```

```
Compilation date                                        : Tue Nov 24 16:11:24 PST 2015
Compiler                                                : gfortran
Compiler options                                        : -c -O3 -fbacktrace -fsign-zero -ffree-line-length-none
Executable                                              : /Users/SAFinsterle/itough2/Executable/itough2_geot


--- End of iTOUGH2 input job:   171 lines read,    0.04 CPU-seconds used


***********************************************************************************************************************
                                                  OUTPUT
***********************************************************************************************************************

LEVENBERG-MARQUARDT ALGORITHM

I  = NEW ITERATION        J  = JACOBIAN            S  = STEP       U  = UNSUCCESSFUL STEP
PS = PARAMETER SELECTION   PU = PARAMETER UPDATE    B  = BOUNDS     M  = MESSAGE

----------------------------------------------------------------------------------------------------------
ITER TOUGH2 OBJ FUNC. MAX. RESID. EQU. STWF no-react-d CFACT no-react- STWF no-react-d CFACT no-react-
----------------------------------------------------------------------------------------------------------
>I  0    1 4.08304E+00 2.01113E+00   17    4.439580E-02    2.070920E+00    3.698070E-02    4.991630E+00
 Finite-difference update of Jacobian matrix (   4 active parameters)
 J  1 Gradient    =   1.24654E+02 (forward)
 ----------------------------------------------------------------------
 S    Step size    =   6.15390E-01    Scaled step size =  6.153899E-05
 DOF  Objective function reduced by  59.95%
 SVD  Singular values of (JT*P*J)  :      2.900222E+05    5.906202E+03    8.005029E+05    1.449845E+04
 PU   Log(LP)=  0. Parameter update:     3.241561E-04   -8.520606E-03    3.068305E-03   -6.153231E-01
>I  1    6 1.63539E+00 7.81244E-01   17    4.471996E-02    2.062399E+00    4.004901E-02    4.376307E+00
 Finite-difference update of Jacobian matrix (   4 active parameters)
 J  2 Gradient    =   3.45730E+01 (forward)
 ----------------------------------------------------------------------
 S    Step size    =   1.08562E+00    Scaled step size =  1.085617E-04
 DOF  Objective function reduced by  94.16%
 SVD  Singular values of (JT*P*J)  :      2.763737E+05    3.501090E+03    2.491319E+05    8.682950E+03
 PU   Log(LP)= -1. Parameter update:     4.140909E-03   -2.644320E-02    2.118381E-03   -1.085285E+00
>I  2   11 9.54608E-02 3.97134E-02   13    4.886086E-02    2.035956E+00    4.216739E-02    3.291022E+00
 Finite-difference update of Jacobian matrix (   4 active parameters)
 J  3 Gradient    =   2.25291E+01 (forward)
 ----------------------------------------------------------------------
 S    Step size    =   1.86047E-01    Scaled step size =  1.860472E-05
 DOF  Objective function reduced by  96.36%
 SVD  Singular values of (JT*P*J)  :      1.648767E+05    1.577272E+04    3.953195E+05    5.207239E+03
 PU   Log(LP)= -2. Parameter update:     1.935532E-03    6.999766E-02   -6.243453E-03   -1.722532E-01
```

```
>I  3   16 3.47492E-03 1.80245E-03   13    5.079640E-02    2.105954E+00    3.592393E-02    3.118769E+00
 Finite-difference update of Jacobian matrix (   4 active parameters)
 J  4 Gradient     =   4.28049E+00 (forward)
 -----------------------------------------------------------------
 S    Step size    =   3.84520E-02    Scaled step size =  3.845203E-06
 DOF  Objective function increased by   55.85%
 U      1. unsuccessful step!           S(k+1)/S(k) =  1.558452E+00
 S    Step size    =   3.69605E-02    Scaled step size =  3.696052E-06
 DOF  Objective function increased by   45.54%
 U      2. unsuccessful step!           S(k+1)/S(k) =  1.455404E+00
 S    Step size    =   1.59025E-02    Scaled step size =  1.590255E-06
 DOF  Objective function reduced by   61.76%
 SVD  Singular values of (JT*P*J)  :       1.172441E+05    1.148793E+04    3.794931E+05    2.501232E+03
 PU   Log(LP)= -1. Parameter update:      7.348901E-04   -1.936514E-03   -1.147294E-03    1.572528E-02
>I  4   23 1.32868E-03 5.03672E-04   17    5.153129E-02    2.104017E+00    3.477664E-02    3.134494E+00
 Finite-difference update of Jacobian matrix (   4 active parameters)
 J  5 Gradient     =   1.90697E+00 (forward)
 -----------------------------------------------------------------
 S    Step size    =   2.45019E-02    Scaled step size =  2.450194E-06
 DOF  Objective function reduced by   94.76%
 SVD  Singular values of (JT*P*J)  :       3.779933E+05    7.438054E+03    2.385586E+05    1.291286E+04
 PU   Log(LP)= -1. Parameter update:     -4.651804E-04   -8.836776E-04    8.397441E-06   -2.448158E-02
>I  5   28 6.95660E-05 2.95949E-05   13    5.106611E-02    2.103134E+00    3.478504E-02    3.110013E+00
 Finite-difference update of Jacobian matrix (   4 active parameters)
 J  6 Gradient     =   1.94403E+00 (forward)
 -----------------------------------------------------------------
 S    Step size    =   3.22604E-03    Scaled step size =  3.226037E-07
 DOF  Objective function increased by   84.59%
 U      1. unsuccessful step!           S(k+1)/S(k) =  1.845881E+00
 S    Step size    =   2.85531E-03    Scaled step size =  2.855308E-07
 DOF  Objective function increased by   60.92%
 U      2. unsuccessful step!           S(k+1)/S(k) =  1.609232E+00
 S    Step size    =   1.64948E-03    Scaled step size =  1.649479E-07
 DOF  Objective function increased by    1.53%
 U      3. unsuccessful step!           S(k+1)/S(k) =  1.015319E+00
 CS   Step size    =   2.23687E-04    Scaled step size =  2.236867E-08 Step tolerance =  1.0E-09 --> Terminate!
```

```
****************************************************************************************************
                                      SENSITIVITY ANALYSIS
****************************************************************************************************

Element Sij of the scaled sensitivity matrix is the partial derivative of the calculated system response zi
with respect to parameter pj, scaled by inverses of the respective standard deviations:
```

$$S_{ij} = \frac{dz_i \; * \; \sigma(p_j)}{dp_j \; * \; \sigma(z_i)}$$

```
        TIME   #  OBSERVATION       STWF no-react-d CFACT no-react- STWF no-react-d CFACT no-react-        TOTAL
0.00000E+00    5  CLUSTER 1.1         103576.84855      5132.99821        -0.00000        -0.00000  108709.84676
0.00000E+00    6  CLUSTER 1.2         256245.21317      5680.04305        -0.00001        -0.00000  261925.25623
0.00000E+00    7  CLUSTER 1.3          70174.86719       529.74012        -0.00023        -0.00000   70704.60754
0.00000E+00    8  CLUSTER 1.4          59818.79659      1960.42163        -0.00012        -0.00000   61779.21834
0.00000E+00    9  CLUSTER 2.1          46641.84353      4996.18329        -0.00000        -0.00000   51638.02682
0.00000E+00   10  CLUSTER 2.2         135780.44515      9621.32655        -0.00000        -0.00000  145401.77170
0.00000E+00   11  CLUSTER 4.1          66902.47899       840.73242         0.00000        -0.00000   67743.21142
0.00000E+00   12  CLUSTER 1.1              0.00012        -0.00001    139585.07751      3554.33501  143139.41264
0.00000E+00   13  CLUSTER 1.2             -0.00018        -0.00001    424348.36509      2724.05755  427072.42283
0.00000E+00   14  CLUSTER 1.3              0.00007         0.00000    115440.98235       256.27758  115697.26001
0.00000E+00   15  CLUSTER 1.4             -0.00001        -0.00000     87204.15847      1055.33055   88259.48903
0.00000E+00   16  CLUSTER 2.1             -0.00000        -0.00000    106267.72200      4613.43882  110881.16082
0.00000E+00   17  CLUSTER 2.2             -0.00000         0.00000    211670.55208      8236.38193  219906.93401
0.00000E+00   18  CLUSTER 4.1              0.00000        -0.00000    110217.10717       -23.69909  110240.80626
0.00000E+00   19  CLUSTER 3.1           8757.67355       219.98725     10880.91281       116.92548   19975.49909
0.00000E+00   20  CLUSTER 3.2           7454.79066       234.23447     45685.51801      -149.11441   53523.65756
0.00000E+00   21  CLUSTER 3.3          -1299.80496        -0.58112      1879.04149        42.90243    3222.32999
0.00000E+00   22  CLUSTER 3.4          54418.26035      5829.17789     62291.00029      4692.57781  127231.01633
-------------------------------------------------------------------------------------------------------------
                                   STWF no-react-d CFACT no-react- STWF no-react-d CFACT no-react-        TOTAL
-------------------------------------------------------------------------------------------------------------
Parameter variation sigma(p)         10000.00000     10000.00000     10000.00000     10000.00000
-------------------------------------------------------------------------------------------------------------
Total from data  CLUSTER 1.1            103576.8          5133.0             0.0             0.0     108709.8
Total from data  CLUSTER 1.2            256245.2          5680.0             0.0             0.0     261925.3
Total from data  CLUSTER 1.3             70174.9           529.7             0.0             0.0      70704.6
Total from data  CLUSTER 1.4             59818.8          1960.4             0.0             0.0      61779.2
Total from data  CLUSTER 2.1             46641.8          4996.2             0.0             0.0      51638.0
Total from data  CLUSTER 2.2            135780.4          9621.3             0.0             0.0     145401.8
Total from data  CLUSTER 4.1             66902.5           840.7             0.0             0.0      67743.2
```

```
Total from data  CLUSTER 1.1              0.0          0.0      139585.1        3554.3      143139.4
Total from data  CLUSTER 1.2              0.0          0.0      424348.4        2724.1      427072.4
Total from data  CLUSTER 1.3              0.0          0.0      115441.0         256.3      115697.3
Total from data  CLUSTER 1.4              0.0          0.0       87204.2        1055.3       88259.5
Total from data  CLUSTER 2.1              0.0          0.0      106267.7        4613.4      110881.2
Total from data  CLUSTER 2.2              0.0          0.0      211670.6        8236.4      219906.9
Total from data  CLUSTER 4.1              0.0          0.0      110217.1          23.7      110240.8
Total from data  CLUSTER 3.1           8757.7        220.0       10880.9         116.9       19975.5
Total from data  CLUSTER 3.2           7454.8        234.2       45685.5         149.1       53523.7
Total from data  CLUSTER 3.3           1299.8          0.6        1879.0          42.9        3222.3
Total from data  CLUSTER 3.4          54418.3       5829.2       62291.0        4692.6      127231.0
---------------------------------------------------------------------------------------------------
Total parameter influence            811072.0      35046.4     1315471.4       25466.0
===================================================================================================
```

ERROR ANALYSIS

****

```
Error analysis is based on >>> a posteriori <<< variance:      0.0000039


Covariance(L+D)/Correlation(U) Matrix of Estimated Parameters
-------------------------------------------------------------
                STWF no-react-d CFACT no-react- STWF no-react-d CFACT no-react-
STWF no-react-d    1.07991E-08          -0.826         -0.071           0.136
CFACT no-react-   -2.07462E-07     5.84598E-06          0.109          -0.212
STWF no-react-d   -3.71008E-10     1.32208E-08     2.51444E-09          -0.691
CFACT no-react-    3.40529E-08    -1.23587E-06    -8.35095E-08     5.81489E-06


Matrix of Pairwise Correlations
-------------------------------
                STWF no-react-d CFACT no-react- STWF no-react-d CFACT no-react-
STWF no-react-d       1.000          -0.823         -0.021          -0.066
CFACT no-react-      -0.823           1.000         -0.047          -0.162
STWF no-react-d      -0.021          -0.047          1.000          -0.687
CFACT no-react-      -0.066          -0.162         -0.687           1.000
```

```
Standard Deviations
-------------------
A PRIORI     : Uncertainty of prior information
CONDITIONAL  : Estimation uncertainty assuming all other parameters are perfectly known
MARGINAL     : Estimation uncertainty (accounts for parameter correlations)
C/M          : Ratio of conditional over marginal estimation uncertainties (measure of parameter independence)
1-M/P        : Relative parameter error reduction (negative may indicate inconsistency between
               prior information and estimate)


PARAMETER         BEST ESTIMATE      A PRIORI      CONDITIONAL       MARGINAL              C/M           1-M/P
STWF no-react-d    3.47850E-02    1.00000E+04    3.62062E-05    5.01442E-05            0.722           1.000
CFACT no-react-    3.11001E+00    1.00000E+04    1.70843E-03    2.41141E-03            0.708           1.000
STWF no-react-d    5.10661E-02    1.00000E+04    5.84626E-05    1.03919E-04            0.563           1.000
CFACT no-react-    2.10313E+00    1.00000E+04    1.34056E-03    2.41785E-03            0.554           1.000


Correlation Chart
-----------------


-1.0    -0.8    -0.6    -0.4    -0.2     0.0                 0.0     0.2     0.4     0.6     0.8     1.0
  |-------|-------|-------|-------|-------|     PARAMETER       |-------|-------|-------|-------|-------|

             |-----------------------|-|  STWF no-react-d  |--|
             |                       |                        |
             |-------------------|----|-|  CFACT no-react-  |--||
                                 |    |                        ||
         |-----------------------|----|-|  STWF no-react-d  |--||
         |                       |                            |
         |-----------------------|------|  CFACT no-react-  |--|
```
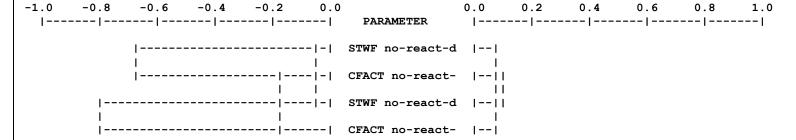
```
Eigenanalysis of Covariance Matrix (R-Mode Factor Analysis)
-----------------------------------------------------------
Performance index :  5.063E-03
Condition number  :  5.397E+03


Eigenvalues
-----------
                                 1          2          3          4
  1 Eigenvalue    :         7.071E-06  4.598E-06  3.416E-09  1.310E-09


Eigenvectors
-----------
                                 1          2          3          4
  1 STWF no-react-d        7.120E-01   7.013E-01   3.584E-02   1.567E-03
  2 CFACT no-react-       -7.017E-01   7.123E-01   1.463E-03   1.457E-02
  3 STWF no-react-d       -2.431E-02  -2.643E-02   9.991E-01   2.107E-02
  4 CFACT no-react-        9.623E-03  -1.092E-02  -2.113E-02   9.997E-01
```

****
                                  RESIDUAL ANALYSIS
****

```
RESIDUAL : Measured - computed
BC       : Box-Cox transformed data
C.O.F.   : Relative contribution to final objective function
STD. DEV.: A posteriori standard deviation of calculated system response
Yi       : Local reliability or influence; observations with Yi < 0.25 are poorly controlled
Wi       : Studentized residual; if abs(Wi) > u(0.95) = 1.96 observation is potential outlier
DWi      : Data-Worth Analysis: Worth of potential and/or existing calibration data [-]
           Metric No. 1:  1-f(C+)/f(C) or 1-f(C)/f(C-), where f(C) = trace(Cpp)
           Changes in covariance matrix Cpp are caused by adding (+) potential or removing (-) existing
           calibration data points
```

# OBSERVATION	AT TIME [sec]	MEASURED	COMPUTED	RESIDUAL	WEIGHT	C.O.F	STD. DEV.	Yi		Wi	DWi
1 STWF no-react-d		4.439E-02	5.106E-02	-6.670E-03	1.00E-04	0.000	1.039E-04				0.000
2 CFACT no-react-		2.070E+00	2.103E+00	-3.221E-02	1.00E-04	0.000	2.418E-03				0.000
3 STWF no-react-d		3.698E-02	3.478E-02	2.195E-03	1.00E-04	0.000	5.014E-05				0.000
4 CFACT no-react-		4.991E+00	3.110E+00	1.881E+00	1.00E-04	0.051	2.411E-03				0.000
1 CLUSTER 1.1	SATURAT MEDI	0.000E+00	5.201E-04	-5.201E-04	2.82E+00	3.112	2.482E-04	0.87		-0.00	0.020
2 CLUSTER 1.2	SATURAT MEAN	0.000E+00	7.307E-04	-7.307E-04	2.82E+00	6.141	6.059E-04	0.24	*	-0.00	0.272

```
 3   CLUSTER 1.3    SATURAT SIGM  0.000E+00  3.536E-04 -3.536E-04  1.00E+00  0.180  6.276E-04 0.90     -0.00 0.032
 4   CLUSTER 1.4    SATURAT RMSE  0.000E+00  6.516E-04 -6.516E-04  1.00E+00  0.610  3.528E-04 0.97     -0.00 0.000
 5   CLUSTER 2.1    SPREAD  MEAN  0.000E+00  4.192E-01 -4.192E-01  5.00E-03  6.317  1.705E-01 0.81     -0.00 0.099
 6   CLUSTER 2.2    SPREAD  SIGM  0.000E+00  1.232E-01 -1.232E-01  3.00E-02 19.665  4.692E-02 0.49     -0.01 0.277
 7   CLUSTER 4.1    OPTIM   MEAS  0.000E+00  2.565E-02 -2.565E-02  1.00E-02  0.095  5.397E-02 0.92     -0.00 0.019
 8   CLUSTER 1.1    SATURAT MEDI  0.000E+00  3.267E-04 -3.267E-04  2.82E+00  1.228  2.224E-04 0.90     -0.00 0.021
 9   CLUSTER 1.2    SATURAT MEAN  0.000E+00  1.923E-03 -1.923E-03  2.82E+00 42.542  6.152E-04 0.22  *  -0.01 0.285
10   CLUSTER 1.3    SATURAT SIGM  0.000E+00  1.698E-03 -1.698E-03  1.00E+00  4.147  5.380E-04 0.93     -0.00 0.016
11   CLUSTER 1.4    SATURAT RMSE  0.000E+00  1.046E-03 -1.046E-03  1.00E+00  1.575  3.197E-04 0.97     -0.00 0.000
12   CLUSTER 2.1    SPREAD  MEAN  0.000E+00  2.353E-01 -2.353E-01  5.00E-03  1.990  1.676E-01 0.82     -0.00 0.085
13   CLUSTER 2.2    SPREAD  SIGM  0.000E+00  8.389E-02 -8.389E-02  3.00E-02  9.105  4.898E-02 0.44     -0.00 0.327
14   CLUSTER 4.1    OPTIM   MEAS  0.000E+00  9.373E-02 -9.373E-02  1.00E-02  1.263  5.566E-02 0.92     -0.00 0.021
15   CLUSTER 3.1    GLOBAL  ESTI  0.000E+00  5.946E-03 -5.946E-03  5.00E-03  0.001  1.378E-02 1.00     -0.00 0.000
16   CLUSTER 3.2    GLOBAL  OTHE  0.000E+00  5.408E-02 -5.408E-02  8.66E-03  0.315  3.000E-02 0.98     -0.00 0.052
17   CLUSTER 3.3    GLOBAL  RANG  0.000E+00  1.414E-02 -1.414E-02  5.00E-03  0.007  2.973E-03 1.00     -0.00 0.000
18   CLUSTER 3.4    GLOBAL  CROS  0.000E+00  1.300E-01 -1.300-01   8.25E-03  1.655  1.458E-01 0.63     -0.00 0.175


Residual Plots
--------------


       RESIDUAL      --------------------
    -3.267E-04      | 8                 |
    -4.688E-02      |17                 |
    -9.343E-02      | 163               |
    -1.400E-01      |    146            |
    -1.865E-01      |     18            |
    -2.331E-01      |                   |
    -2.796E-01      |          12       |
    -3.262E-01      |                   |
    -3.727E-01      |                   |
    -4.193E-01      |                  5|
                    --------------------
             3.267E-04           4.193E-01
                 GEOT CLUSTERING [-]
```

```
Summary of Residual Analysis
----------------------------
Max weighted residual at observation   :             13
Max weighted residual                  :     -5.4401E-03
Max residual                           :     -1.9234E-03
Number of poorly controlled observations:             2
Number of large normalized residuals   :              0
Max normalized residual at observation :             13
Max normalized residual                :           0.01
Probable size of maximum error         :      8.8901E-03


Iteration Statistics
--------------------
Number of iterations                   :              5
Number of forward runs                 :             35
Number of non-TOUGH2 runs              :             35


Control Measures
----------------
Trace (P*QLL) : n   =   4              :           4.00
Sum   (Yi)    : m-n =  14              :          14.00


Objective Function
------------------
Initial value of objective function    :      4.0830E+00                                    5869302.20 %
Minimum value of objective function    :      6.9566E-05                                     100.00 %


?!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
ESTIMATED PARAMETER  V/L/F   ROCKS PAR INITIAL GUESS   BEST ESTIMATE       STANDARD DEVIATIONS       SENSITIVITY
                                                                      A PRIORI  MARGINAL    C/M  OUTPUT    OBJFUNC
STWF no-react-d    VALUE    no-re   1   4.43958E-02       5.107E-02 1.00E+04 1.039E-04  0.563  811072.0  8624.410
CFACT no-react-    VALUE    no-re   2   2.07092E+00       2.103E+00 1.00E+04 2.418E-03  0.554   35046.4   599.099
STWF no-react-d    VALUE    no-re   1   3.69807E-02       3.479E-02 1.00E+04 5.014E-05  0.722 1315471.4 17404.625
CFACT no-react-    VALUE    no-re   2   4.99163E+00      3.1100E+00 1.00E+04 2.411E-03  0.708   25466.0   513.309
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!


---    532nd iTOUGH2 run stopped normally on 27-Nov-15  14:35 ---  CPU time used =        1.23 sec.


---     0 error(s) and  0 warning(s) detected
```

Figure 10. iGeoT output file *igeot.out*.

```
**********************************************
* Program iGeoT Version 2.1    LBNL/ESD 2016 *
**********************************************


Artificial geothermal water at 250 C, 3 bar CO2  (Equilibrate SV Phipps-2 water)
***************************************************************************


Geothermometry calculations using the flagged minerals below


Water  1    ID: no-react-degas                              stwf = 0.051 cfact = 2.106  stwf iter = 0
-------------------------------------------------------------------------------------
Classical Geothermometers    T(C)  (for info only, reconstructed water, zero if no data)
---------------------------------
  Quartz  (Four&Pott82) :    228.7  (no steam loss)
  Am.Silica    (Four77) :    101.9
  Chalcedony   (Four77) :    213.8
  Na-K-Ca (Four&True73) :    237.7
  Na-K         (Gigg88) :    257.4  (Four79)  244.1
  K-Mg         (Gigg88) :    251.0
  Na-Li   (Foui&Mich81) :      0.0


---------------------------------
Multicomponent Geothermometer T(C)
---------------------------------
  T(C) cross average   :    250.0   T cross SDEV :   0.027        T range  :   250.0 - 250.0
  T(C) at minimum RMED :    250.0   minimum RMED :   0.000        T spread :     0.1
  T(C) at minimum RMSE :    250.0   minimum RMSE :   0.000
  T(C) at minimum SDEV :    250.0   minimum SDEV :   0.000
  T(C) at minimum MEAN :    250.0   minimum MEAN :   0.000
  T(C) weighted average :   250.0   number of minerals selected for T estimation :  8
                                    optimgeot(1) = Trmed-Tstatav            :   0.0162
                                    optimgeot(2) = RMED/nmina               :   0.0000


Temperature (C) --->    100.00    110.00    120.00    130.00   ...... 240.00    250.00    260.00
Gas sat. P(bar) --->      6.63      7.43      8.31      9.28   ......  39.99     46.08     52.99
Iterations                 11         4         4         4   ......      6         6         6
```

```
pH                      5.27      5.33      5.39      5.45   ......   6.45      6.57      6.71


RMED                    0.67      0.63      0.58      0.54   ......   0.08      0.00      0.09
RMSE                    2.86      2.60      2.35      2.11   ......   0.15      0.00      0.14
SDEV                    2.45      2.21      1.98      1.75   ......   0.10      0.00      0.09
MEAN                    1.71      1.58      1.44      1.33   ......   0.11      0.00      0.12


              Scaled saturation indices:  * (or **) if......
microcli        **  0.18      0.23      0.28      0.33   ......   0.08      0.00     -0.09
heulandi        **  0.38      0.41      0.44      0.47   ......   0.09     -0.00     -0.09
albit-lo        ** -0.16     -0.08     -0.00      0.07   ......   0.06      0.00     -0.07
anhydrit        ** -1.82     -1.68     -1.55     -1.42   ......  -0.10      0.00      0.10
quartz          *   0.81      0.74      0.66      0.59   ......   0.04      0.00     -0.04
calcite         *  -2.39     -2.22     -2.06     -1.90   ......  -0.16     -0.00      0.16
fluorite        *  -0.53     -0.52     -0.50     -0.49   ......  -0.05      0.00      0.05
clchlore        *  -7.44     -6.74     -6.05     -5.39   ......  -0.34     -0.00      0.33


                  Mole fractions at saturation
h2o(g)            0.167E+00 0.210E+00 0.260E+00 0.316E+00 ......0.867E+00 0.890E+00 0.909E+00 0
co2(g)            0.833E+00 0.790E+00 0.740E+00 0.684E+00 ......0.133E+00 0.110E+00 0.912E-01 0


                  Partial pressures (bar)
h2o(g)            0.111E+01 0.156E+01 0.216E+01 0.293E+01 ......0.347E+02 0.410E+02 0.482E+02 0
co2(g)            0.553E+01 0.587E+01 0.615E+01 0.635E+01 ......0.533E+01 0.508E+01 0.483E+01 0



Water   2    ID: no-react-degas2                       stwf = 0.034 cfact = 3.137  stwf iter = 0
--------------------------------------------------------------------------------------------------
Classical Geothermometers    T(C)  (for info only, reconstructed water, zero if no data)
----------------------------------
  Quartz  (Four&Pott82) :    229.5  (no steam loss)
  Am.Silica   (Four77) :    102.7
  Chalcedony  (Four77) :    214.8
  Na-K-Ca (Four&True73) :    237.8
  Na-K        (Gigg88) :    257.4  (Four79)  244.1
  K-Mg        (Gigg88) :    251.3
  Na-Li   (Foui&Mich81) :      0.0
```

```
--------------------------------
Multicomponent Geothermometer T(C)
--------------------------------
  T(C) cross average    :     250.0   T cross SDEV :    0.917        T range   :   248.2 - 251.1
  T(C) at minimum RMED  :     250.1   minimum RMED :    0.005        T spread :      2.9
  T(C) at minimum RMSE  :     249.9   minimum RMSE :    0.005
  T(C) at minimum SDEV  :     249.8   minimum SDEV :    0.001
  T(C) at minimum MEAN  :     250.0   minimum MEAN :    0.005
  T(C) weighted average :     249.9   number of minerals selected for T estimation :  8
                                      optimgeot(1) = Trmed-Tstatav                 :  0.1683
                                      optimgeot(2) = RMED/nmina                    :  0.0006


Temperature (C) --->      100.00    110.00    120.00    130.00   ......   240.00    250.00    260.00
Gas sat. P(bar) --->        6.68      7.48      8.36      9.34   ......    40.04     46.13     53.04
Iterations                    12         4         4         5   ......        6         6         6


 pH                         5.27      5.33      5.39      5.45   ......     6.45      6.57      6.71


 RMED                       0.67      0.62      0.58      0.54   ......     0.09      0.00      0.09
 RMSE                       2.86      2.60      2.35      2.10   ......     0.14      0.01      0.15
 SDEV                       2.45      2.21      1.98      1.75   ......     0.10      0.00      0.10
 MEAN                       1.71      1.57      1.44      1.33   ......     0.11      0.01      0.12


                  Scaled saturation indices:   * (or **) if......
 anhydrit          **  -1.81     -1.68     -1.54     -1.41   ......    -0.10      0.00      0.10
 heulandi          **   0.38      0.41      0.44      0.47   ......     0.09      0.00     -0.09
 quartz            **   0.82      0.74      0.67      0.60   ......     0.04      0.00     -0.03
 microcli          **   0.19      0.23      0.28      0.33   ......     0.08      0.00     -0.08
 albit-lo          *   -0.16     -0.08     -0.00      0.07   ......     0.07      0.00     -0.06
 calcite           *   -2.38     -2.22     -2.05     -1.89   ......    -0.15      0.01      0.16
 clchlore          *   -7.43     -6.73     -6.05     -5.38   ......    -0.33      0.01      0.34
 fluorite          *   -0.52     -0.51     -0.49     -0.48   ......    -0.04      0.01      0.06


                  Mole fractions at saturation
 h2o(g)             0.166E+00 0.209E+00 0.259E+00 0.314E+00 ......0.866E+00 0.889E+00 0.908E+00 0
 co2(g)             0.834E+00 0.791E+00 0.741E+00 0.686E+00 ......0.134E+00 0.111E+00 0.918E-01 0
```

```
                         Partial pressures (bar)
 h2o(g)                     0.111E+01 0.156E+01 0.216E+01 0.293E+01 ......0.347E+02 0.410E+02 0.482E+02 0
 co2(g)                     0.557E+01 0.592E+01 0.620E+01 0.640E+01 ......0.537E+01 0.512E+01 0.487E+01 0




 *******************************************************
 Global optimization data (to use with multiple waters):
    Average estimated T =    250.031  stdev =   0.047248
    Average T other stat=    249.955  stdev =   0.083188
    Average of T range  =    250.020  stdev =   0.023680
    Average T spread    =      1.503  stdev =   2.002454
```

Figure 11. Excerpt of GeoT output file *geot.out* after parameter estimation.

5.3 Mapping the Objective Function using iGeoT in Expert Mode

iGeoT can be run in expert mode to refine the inversion by adjusting the automatically generated control file, or to perform other calculations. To demonstrate a simple application, the control file *igeot.inp* shown in **Figure 12** instructs iGeoT to map the objective function in the three-dimensional parameter space. This iGeoT input file is a slightly modified version of file *geot.iGeoT*, which was created by running iGeoT in automatic mode (see Section 5.2). The following changes were made (highlighted in red): (1) A parameter hypercube was defined by setting reasonable lower and upper bounds for the first three parameters using command `>>>> RANGE`; (2) the fourth parameter was deactivated by adding command `>>>> INACTIVE`; (3) the prior value for the fourth parameter was set to its best estimate from the previous inversion; and (4) the `>>> GRID SEARCH` option was invoked in the `> COMPUTATION` block, dividing each of the three parameters axes into 19 intervals (i.e., 20 points). The same GeoT input file as in the previous two examples is used (see **Figure 6**).

The problem is run on Linux by typing the command line:

`igeot igeot.inp geot.inp &`

or by simply typing the name of the executable under Windows and typing <return> when prompted for input file names, which results in these default file names being used.

iGeoT evaluates the objective function (i.e., the sum of the squared, weighted clustering measures) at $20 \times 20 \times 20 = 8000$ points in the parameter space. A few CPU minutes are needed for this exhaustive evaluation of the parameter space. A visualization of the results is shown in **Figure 13**. The objective function exhibits a complex, albeit rather smooth, topology in the three-dimensional parameter space. The minimum is near the parameter set (STWF1, CFACT1, STWF2) = (0.052, 2.10, 0.035).

Note that the derivative-based minimization algorithm discussed in Section 5.2 required only 35 GeoT runs to identify the minimum in the four-dimensional parameter space, requiring on the order of 1 CPU second.

```
File *samGEOT.iGeoT* was automatically generated by iGeoT.

GeoT thermodynamic database FILE: tk-slt.h06_jan14.dat

> PARAMETER

  >> GeoT              STWF
     >>> WATER         : no-react-degas
         >>>> VALUE
         >>>> PRIOR    :  0.443958E-01
         >>>> RANGE    :  0.0 0.1
         <<<<
     <<<

  >> GeoT              CFACT
     >>> WATER         : no-react-degas
         >>>> VALUE
         >>>> PRIOR    :  0.207092E+01
         >>>> RANGE    :  1.0 5.0
         <<<<
     <<<

  >> GeoT              STWF
     >>> WATER         : no-react-degas2
         >>>> VALUE
         >>>> PRIOR    :  0.369807E-01
         >>>> RANGE    :  0.0 0.1
         <<<<
     <<<

  >> GeoT              CFACT
     >>> WATER         : no-react-degas2
         >>>> VALUE
         >>>> PRIOR    :  3.1100E+00
         >>>> DEVIATION :  0.100000E+05
         >>>> INACTIVE
         <<<<
     <<<
  <<

> OBSERVATION

  >> GeoT
     >>> CLUSTER 1.1 - SATURATION MEDIAN WATER: no-react-degas
         >>>> WEIGHT: 2.82843
         <<<<

     >>> CLUSTER 1.2 - SATURATION MEAN   WATER: no-react-degas
         >>>> WEIGHT: 2.82843
         <<<<
```

```
   >>> CLUSTER 1.3 - SATURATION SIGMA  WATER: no-react-degas
       >>>> WEIGHT: 1.00000
       <<<<

   >>> CLUSTER 1.4 - SATURATION RMSE   WATER: no-react-degas
       >>>> WEIGHT: 1.00000
       <<<<

   >>> CLUSTER 2.1 - SPREAD MEAN       WATER: no-react-degas
       >>>> WEIGHT: 0.00500
       <<<<

   >>> CLUSTER 2.2 - SPREAD SIGMA      WATER: no-react-degas
       >>>> WEIGHT: 0.03000
       <<<<

   >>> CLUSTER 4.1 - OPTIMIZATION      WATER: no-react-degas
       >>>> WEIGHT: 0.01000
       <<<<

   >>> CLUSTER 1.1 - SATURATION MEDIAN WATER: no-react-degas2
       >>>> WEIGHT: 2.82843
       <<<<

   >>> CLUSTER 1.2 - SATURATION MEAN   WATER: no-react-degas2
       >>>> WEIGHT: 2.82843
       <<<<

   >>> CLUSTER 1.3 - SATURATION SIGMA  WATER: no-react-degas2
       >>>> WEIGHT: 1.00000
       <<<<

   >>> CLUSTER 1.4 - SATURATION RMSE   WATER: no-react-degas2
       >>>> WEIGHT: 1.00000
       <<<<

   >>> CLUSTER 2.1 - SPREAD MEAN       WATER: no-react-degas2
       >>>> WEIGHT: 0.00500
       <<<<

   >>> CLUSTER 2.2 - SPREAD SIGMA      WATER: no-react-degas2
       >>>> WEIGHT: 0.03000
       <<<<

   >>> CLUSTER 4.1 - OPTIMIZATION      WATER: no-react-degas2
       >>>> WEIGHT: 0.01000
       <<<<


 Global clustering measures; number of waters:  2

   >>> CLUSTER 3.1 - GLOBAL ESTIMATED
```

```
              >>>> WEIGHT: 0.00500
              <<<<

      >>> CLUSTER 3.2 - GLOBAL OTHER
              >>>> WEIGHT: 0.00866
              <<<<

      >>> CLUSTER 3.3 - GLOBAL RANGE
              >>>> WEIGHT: 0.00500
              <<<<

      >>> CLUSTER 3.4 - GLOBAL CROSS
              >>>> WEIGHT: 0.00825
              <<<<
      <<<
  <<

> COMPUTATION

  >> OPTION
     >>> GRID SEARCH: 19
     <<<
  <<
<
```

Figure 12.   iGeoT input file *igeot.inp* for mapping objective function in three-dimensional parameter space.
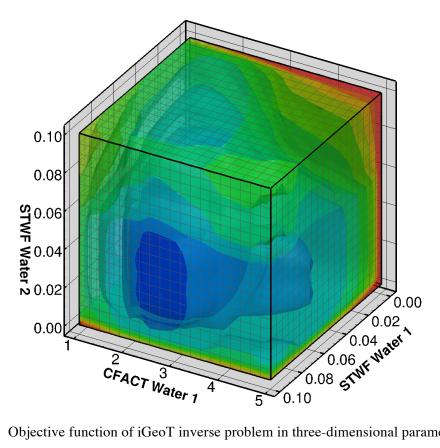
Figure 13. Objective function of iGeoT inverse problem in three-dimensional parameter space.

6. CONCLUDING REMARKS

Multicomponent geothermometry is a powerful approach to estimate temperatures in geothermal reservoirs based on the chemical composition of sampled fluid mixtures. The program GeoT [*Spycher et al.*, 2014, 2016a and 2016b] provides such estimates by minimizing the clustering of multiple saturation index lines about the equilibrium point. However, this clustering may be biased if the water sample underwent degassing, and/or it is concentrated or diluted, and/or the dissolved mineral concentrations are in error.

iGeoT uses automatic parameter estimation techniques to estimate these unknown or uncertain input parameters to multicomponent geothermometry. A nonlinear least-squares problem is solved, where the difference of multiple clustering measures from their optimal value is minimized by automatically adjusting the parameters of interest.

iGeoT can be run in forward mode just as GeoT without parameter estimation, or in two additional modes for parameter estimation, referred to as Automatic and Expert modes. In the automatic mode, the user only needs to identify the parameters that shall be estimated; iGeoT then automatically formulates the related inverse problem and solves it. In expert mode, the user is given the flexibility and power of all the features implemented in the underlying iTOUGH2 optimization toolset.

Illustrative examples of have been provided to demonstrate the usage and results of iGeoT applications. In particular, it was demonstrated that the correct reservoir temperature can be identified if uncertain geothermometry input parameters are estimated using iGeoT.

7. ACKNOWLEDGMENT

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